Collected Algorithms from ACM

Volume I
Algorithms 1-220

A collection of the first 220 ACM Algorithms, including Certifications, Remarks, and Translations from the Algorithms Department of Communications of the ACM, 1960-1963.

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Preface

The Algorithms department of Communications of the ACM (CACM) was established in February 1960, with J. H. Wegstein as editor, for the purpose of publishing algorithms, consisting of procedures and programs, in the Algol language. In 1975 the publication of ACM algorithms material was transferred to ACM Transactions on Mathematical Software (TOMS). A wide variety of algorithms have been published and many of them have been used heavily—either in original form or as translated into other languages. Recognizing the general acceptance of the algorithm material published in CACM and TOMS, the Association for Computing Machinery (ACM) has collected and reprinted the algorithms to make them more readily accessible and more serviceable to a larger group of users.

This collection contains the first 220 algorithms published in the Algorithms department of CACM from 1960 to 1963.

Algorithms 1–220 were originally published as received—without any refereeing whatever. Many of these have since been certified and/or corrected by their authors or by other contributors.

To facilitate the updating and to make this volume convenient to use, an understanding of the page numbering scheme for the algorithms is helpful. The page designation is in a three-part format: the left part is the algorithm number; the middle part is the page number within the algorithm (the first page of each algorithm is P1); and the right part is the number of the revision of that page. All sheets in the original, or first, insertion of an algorithm have "0" for the right part. The first revision of a page will have a page number having the left and middle parts identical with those on the page to be replaced, but the right part will be "R1" instead of "0." The second revision of the same page would read R2, and so on. For example, 123-P2-R1 would mean the first revision of page 2 of Algorithm 123.

Information on submitting algorithms for publication may be found in the introductory section located in the front of the current loose-leaf collection. Included in this material is a cumulative index to all the algorithms published since 1960 as well as the ACM Algorithms Policy, which guides the publication of all algorithms submitted to ACM.

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1. QUADI

R. J. Herbold
National Bureau of Standards, Washington 25, D. C.

```
comment     QuadI is useful when integration of several functions of same limits at same time using same
            point rule is desired. The interval (a,b) is divided into m equal subintervals for an n-point
            quadrature integration. p is the number of functions to be integrated. w_k and u_k are normalized
            weights and abscissas respectively, where k=1,2,3,···,n. u_k must be in ascending order.
            P(B,j) =: (c) is a procedure which must be supplied by the programmer. It evaluates (c) the
            function (as indicated by j) for B. I_j is the result of integration for function j.;
procedure   QuadI (a,b,m,n,p,w_k,u_k,P(B,j) =: (c)) =: (Ij)
            begin
QuadI:              h := (b−a)/m
            for     j := 1(1)p  ;  I_j := 0
                    A := a−h/2
            for     i := 1(1)m
L1          begin   A := A+h
            for     k := 1(1)n
L2          begin   B := A+(h/2)×u_k
            for     j := 1(1)p
L3:         begin   P(B,j) =: (c)
                    I_j := I_j+w_k×c    end L3  ;  end L2
                      end L1
            for     j := 1(1)p
                    I_j := (h/2)×I_j
            return
            integer (j,k,i)
            end     QuadI
```

2. ROOTFINDER

J. Wegstein
National Bureau of Standards, Washington 25, D. C.

```
comment     This procedure computes a value of g=x satis-
            fying the equation x=f(x). The procedure calling
            statement gives the function, an initial approxi-
            mation a≠0 to the root, and a tolerance
            paramater ε for determining the number of sig-
            nificant figures in the solution. This accelerated
            iteration or secant method is described by the
            author in Communications, June, 1958.;
procedure   Root(f( ), a, ε ) =: (g)
begin
Root        b := a  ;  c := f(b)  ;  g := c
            if (c=a)  ;  return
            d := a  ;  b := c  ;  e := c
Hob:        c := f(b)
            g := (d×c−b×e)/(c−e−b+d)
            if (abs((g−b)/g)≦ε)  ;  return
            e := c  ;  d := b  ;  b := g  ;  go to Hob
end
```

CERTIFICATION

2. ROOTFINDER, J. Wegstein, *Communications ACM*, February, 1960

Henry C. Thacher, Jr.,* Argonne National Laboratory, Argonne, Illinois

Rootfinder was coded for the Royal-Precision LGP-30 Computer, using an interpretive floating point system with 28 bits of significance. The translation from ALGOL was made by hand. Provision was made to terminate the iteration after ten cycles if convergence had not been secured.

The program was tested against the following functions:

(1)	$f(x) = (x + 1)^{1/3}$	(Root = 1.3247180)
(2)	$f(x) = \tan x$	
(3.α)	$f(x) = 2\pi\alpha + \tan^{-1} x$	(α = 1, 2, 3, 4)
(4.α)	$f(x) = \sinh \alpha x$	(α = −1.2, −0.5, 0.5, 1.2)

Selected results were as follows:

f(x)	α	ϵ	x_{k-1}	x_k	
1	1.3	10^{-7}, 10^{-6}	1.3247233	1.3258637	(1)
1	1.3	10^{-5}		1.3247165	(1)
2	5	10^{-3}	−.4674691	−.36021288	(1, 2)
2	4	10^{-3}	+.84880381	+.69496143	(1, 2)
3.1	1	10^{-5}		7.7252531	
3.2	2	10^{-5}		14.066155	
3.3	3	10^{-5}		20.371026	
3.4	4	10^{-5}		26.665767	

(1) No convergence after 10 iterations. Underlined figures are incorrect.

(2) For this function, f'(0) = 1; so convergence is not to be expected at this root. However, the algorithm did not find any other root.

It should be noted that the convergence criterion used fails for a zero root. The provision to terminate after a given number of cycles is therefore essential. Also, double precision is desirable.

* Work supported by the U. S. Atomic Energy Commission.

REMARK ON ALGORITHM 2
ROOTFINDER (J. Wegstein, *Communications ACM*, February, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

$$\frac{y_k - Y}{y_{k-1} - Y} = \frac{(y_{k-2} - Y)f''}{2(f' - 1) + (y_{k-1} - y_{k-2})f''} + O(y_{k-1} - Y)^3$$

where Y is the desired root, and the derivatives f' and f'' are evaluated there. Convergence is thus second order, provided that $| f'' | | y_{k-1} - Y | < 2 | f' - 1 |$.

The algorithm is, however, somewhat unstable numerically because of the factor $f(y_{k-1}) - f(y_{k-2}) - y_{k-1} + y_{k-2}$ in the denominator.

Experience has shown that the minimum for ϵ is about one half the precision being used. Provision to indicate when round-off errors are causing random oscillations of g would be a desirable addition.

The criterion used for terminating the iteration renders the algorithm unsuitable for a zero root. A preliminary test for a zero root would be desirable. In addition, the algorithm should include provision for exit after a stated number of iterations.

Algorithm 15 appears to offer advantages along these lines.

* Work supported by the U. S. Atomic Energy Commission.

This algorithm has the convergence factor

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

J. H. WILKINSON
National Physical Laboratory, Teddington.

Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the *method* of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \cdots = a_5 = 0$, $a_6 =$

$a_7 = \cdots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^5(x-1)^6(x-2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-44}. Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic. This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, *is a very well-conditioned method of evaluation.* Knowing this, I was able to set a tolerance of 2^{-42} with confidence. If the *same function* had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $|x_{r+1} - x_r|$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$\tan x - x = -n\pi + \frac{x = n\pi + y}{\dfrac{y^3}{3} - \dfrac{y^5}{30} - \cdots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^{60} - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable number of iterations are needed to find the root $x = 1$. Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is use ful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4, that abs(fprt) < abs(x2 × 10), but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on the size of the function and on the size of the remainders r1 and r0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (Comm. ACM June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to *slow* convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root $x = -6.35099\,36103$ and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

[1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150–180.

3. Solution of Polynomial Equation by Bairstow-Hitchcock Method

A. A. Grau
Oak Ridge National Laboratory, Oak Ridge, Tenn.

```
procedure
BAIRSTOW  (n, a[ ], eps0, eps1, eps2, eps3, K) =:
          (m, x[ ], y[ ], nat[ ], ex[ ]);
comment   The Bairstow-Hitchcock iteration is used to find
          successively pairs of roots of a polynomial
          equation of degree n with coefficients a_i
          (i = 0, 1, ···, n) where a_n is the constant term. On
          exit from the procedure, m is the number of pairs
          of roots found, x[i] and y[i]  (i = 1, ···, m) are a
          pair of real roots if nat[i]=1, the real and imagi-
          nary parts of a complex pair if nat[i]=−1, and
          ex[i] indicates which of the following conditions
          was met to exit from the iteration loop in finding
          this pair:
            1. Remainders, r1, r0, become absolutely less
               than eps1.
            2. Corrections, incrp, incrq, become absolutely
               less than eps2.
            3. The ratios, incrp/p, incrq/q, become ab-
               solutely less than eps3.
            4. The number of iterations becomes K.
          In the last case, the pair of roots found is not
          reliable and no further effort to find additional
          roots is made. The quantity eps0 is used as a
          lower bound for the denominator in the expres-
          sions from which incrp and incrq are found.;
begin
integer   (i, j, k, n1, n2, m1)  ;
array     (b, c[0 : n+1])  ;
BAIRSTOW  for i := 0(1)n  ; b_i := a_i
          b_{n+1} := 0  ; n2 := entire((n+1)/2)
            n1 := 2×n2
          for m1 := 1(1)n2  ; begin p := 0  ; q := 0
          for k := 1(1)K  ; begin
step:     for i := 0(1)n1  ; c_i := b_i
          for j := n1−2, n1−4  ; begin
          for i := 0(1)j  ; begin
          c_{i+1} := c_{i+1} − p × c_i
          c_{i+2} := c_{i+2} − q × c_i end end
          r0 := c_{n1}  ; r1 := c_{n1−1}
          s0 := c_{n1−2}  ; s1 := c_{n1−3}
          v0 := −q × s1  ; v1 := s0 − s1 × p
          det0 := v1 × s0 − v0 × s1
          if (abs(det0)<eps0)  ; begin
          p := p+1  ; q := q+1  ; go to step end
          det1 := s0 × r1 − s1 × r0
          det2 := r0 × v1 − v0 × s1
          incrp := det1/det0  ; incrq := det2/det0
          p := p + incrp  ; q := q + incrq
          if (abs (r0) < eps1)  ; begin
          if (abs (r1) < eps1)  ; begin
          ex_{m1} := 1  ; go to next end end
          if (abs (incrp) < eps2)  ; begin
          if (abs (incrq) < eps2)  ; begin
          ex_{m1} := 2  ; go to next end end
          if (abs (incrp/p) < eps3)  ; begin
          if (abs (incrq/q) < eps3)  ; begin
          ex_{m1} := 3  ; go to next end end end
          ex_{m1} := 4
next:     S := p/2  ; T := S² − q
          if (T ≧ 0)  ; begin T := sqrt (T)
          nat_{m1} := 1  ; x_{m1} := S + T
            y_{m1} := S − T end
          if (T < 0)  ; begin nat_{m1} := −1  ; x_{m1} := S
            y_{m1} := sqrt(−T) end
          if (ex_{m1} := 4)  ; go to out
          for j := 0(1) (n1−2)  ; begin
          b_{j+1} := b_{j+1} − p × b_j
          b_{j+2} := b_{j+2} − q × b_j  ; end
          n1 := n1 − 2  ; if  (n1 < 1)
out:      begin m := m1  ; return end
          if (n1 < 3)  ; begin
          m1 := m1 + 1  ; ex_{m1} := 1
          p := b_1/b_0  ; q := b_2/b_0
          go to next end
end end
```

CERTIFICATION

3. Solution of Polynomial Equation by Bairstow-Hitchcock Method, A. A. Grau, *Communications ACM*, February, 1960.

Henry C. Thacher, Jr.,* Argonne National Laboratory, Argonne, Illinois.

Bairstow was coded for the Royal-Precision LGP-30 computer, using an interpretive floating point system (24.2) with 28 bits of significance. The translation from Algol was made by hand.

The following minor corrections were found necessary.

a. det 2 := r0 × v1 − v0 × s1 should be det 2 := r0 × v1 − v0 × r1

b. S := p/2 should be S := −p/2.

After these were made, the program ran smoothly for the following equations:

$x^4 - 3x^3 + 20x^2 + 44x + 43 = 0$ $\quad x = -.97063897 \pm 1.0058076i$

$x = -2.4706390 \pm 4.6405330i$

$x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$

$x = 0.50000000 \pm 0.86602539i$

$x = 1.0000000 \pm 1.0000000i$

$x = 1.5000000 \pm 1.3228756i$

$x^5 + x^4 - 8x^3 - 16x^2 + 7x + 15 = 0$

$x = .000000005,^{**} - 0.99999999$

$x = 3.0000000, 0.99999999$

$x = -2.0000000 \pm 1.0000000i$

With the equation $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ convergence was slow, and full accuracy was not obtained. However, the

equation with reciprocal roots, $2x^5 + 3x^4 + 6x^3 + 5x^2 + 7x + 1 = 0$, converged rapidly.

---

* Work supported by the U. S. Atomic Energy Commission.

** Spurious zero real roots are introduced for equations of odd order.

CERTIFICATION OF ALGORITHM 3 SOLUTION OF POLYNOMIAL EQUATIONS BY BAIRSTOW HITCHCOCK METHOD (A. A. Grau, *Comm. ACM*, February, 1960)

JAMES S. VANDERGRAFT
Stanford University, Stanford, California

Bairstow was coded for the Burroughs 220 computer using the Burroughs ALGOL. Conversion from ALGOL 60 was made by hand on a statement-for-statement basis. The integer declaration had to be extended to include n, k, n, NAT, EX, and the corrections noted in the certification by Henry C. Thacher, Jr., *Communications ACM*, June, 1960, were incorporated.

By selecting the input parameters carefully, all branches of the routine were tested and the program ran smoothly. The following polynomials equations were solved:

$x^6 - 14x^4 + 49x^2 - 36 = 0$, $x = \pm 1.0000000$
$x = \pm 1.9999998$
$x = \pm 3.0000001$

$x^8 - 30x^6 + 273x^4 - 820x^2 + 576 = 0$, $x = \pm 1.0000000$
$x = \pm 2.0000000$
$x = \pm 2.9999999$
$x = \pm 4.0000001$

Several minor errors were found in the certification by Mr. Thacher. The constant term in the first polynomial should be 54 instead of 43, the second pair of roots for that polynomial should be $+ 2.470639 \pm 4.6405330$ i, and the second pair of roots for the second polynomial should be $-1.0 \pm$ i.

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

J. H. WILKINSON
National Physical Laboratory, Teddington.

Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the *method* of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \cdots = a_5 = 0$, $a_6 = a_7 = \cdots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^5(x - 1)^5(x - 2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-44}. Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic. This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, *is a very well-conditioned method of evaluation*. Knowing this, I was able to set a tolerance of 2^{-42} with confidence. If the *same function* had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $| x_{r+1} - x_r |$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$x = n\pi + y$$

$$\tan x - x = -n\pi + \frac{\frac{y^3}{3} - \frac{y^5}{30} - \cdots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^{60} - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable number of iterations are needed to find the root $x = 1$. Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is use ful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4, that abs(fprt) < abs(x2 × 10), but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on the size of the function and on the size of the remainders r1 and r0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (Comm. ACM June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to *slow* convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root $x = -6.35099\ 36103$ and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original

polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

[1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150–180.

CERTIFICATION OF ALGORITHM 3 SOLUTION OF POLYNOMIAL EQUATION BY BARSTOW-HITCHCOCK (A. A. Grau, *Comm. ACM* Feb. 1960)

JOHN HERNDON
Stanford Research Institute, Menlo Park, California

Bairstow was transliterated into BALGOL and tested on the Burroughs 220. The corrections supplied by Thatcher, *Comm. ACM*, June 1960, were incorporated. Results were correct for equations for which the method is suitable. $x^4 - 16 = 0$ is one of those which gave nonsensical results. Seven-digit results were obtained for 12 test equations, one of which was $x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$.

4. BISECTION ROUTINE

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Philadelphia, Pa.

```
comment  This procedure evaluates a function at the end-points
         of a real interval, switching to an error exit (fools
         exit) FLSXT if there is no change of sign. Otherwise
         it finds a root by iterated bisection and evaluation
         at the midpoint, halting if either the value of the
         function is less than the free variable ε or two suc-
         cessive approximations of the root differ by less
         than ε1. ε should be chosen of the order of error in
         evaluating the function (otherwise time would be
         wasted), and ε1 of the order of desired accuracy. ε1
         must not be less than two units in the last place
         carried by the machine or else indefinite cycling will
         occur due to round-off on bisection. Although this
         method is of 0 order, and therefore among the slow-
         est, it is applicable to any continuous function. The
         fact that no differentiability conditions have to be
         checked makes it, therefore, an 'old work-horse'
         among routines for finding real roots which have
         already been isolated. The free variables y1 and y2
         are (presumably) the end-points of an interval within
         which there is an odd number of roots of the real
         function F. α is the temporary exit for the evalua-
         tion of F.;
procedure Bisec(y1, y2, ε, ε1, F( ), FLSXT) =: (x)
begin
Bisec:   i := 1 ; j := 1 ; k := 1 ; x := y2
α:       f := F(x) ; if (abs(f) ≦ ε) ; return
         go to γ1
First val: i := 2 ; f1 := f ; x := y1 ; go to α
Succ val: if (sign(f) = sign(f1)) ; go to δj ; go to ηk
Sec val: j := 2 ; k := 2
Midpoint: x := y1/2 + y2/2 ; go to α
Reg δ:   y2 := x
Precision: if (abs(y1 − y2) ≧ ε1) ; go to Midpoint
         return
Reg η:   y1 := x ; go to Precision
         integer (i, j, k)
         switch γ := (First val, Succ val)
         switch δ := (FLSXT, Reg δ)
         switch η := (Sec val, Reg η)
end Bisec
```

CERTIFICATION OF ALGORITHM 4
BISECTION ROUTINE (S. Gorn, *Comm. ACM*, March 1960)

PATTY JANE RADER,* Argonne National Laboratory, Argonne, Illinois

BISEC was coded for the Royal-Precision LGP-30 computer, using an interpretive floating point system (24.2) with 28 bits of significance.

The following minor correction was found necessary.

α: **go to** γ_1 should be **go to** γ_i

* Work supported by the U. S. Atomic Energy Commission.

After this correction was made, the program ran smoothly for F(x) = cos x, using the following parameters:

y_1	y_2	ϵ	ϵ_1	Results
0	1	.001	.001	FLSXT
0	2	.001	.001	1.5703
1.5	2	.001	.001	1.5703
1.55	2	.1	.1	1.5500
1.5	2	.001	.1	1.5625

These combinations test all loops of the program.

* Work supported by the U. S. Atomic Energy Commission.

5. Bessel Function I, Series Expansion

Dorothea S. Clarke
General Electric Co., FPLD, Cincinnati 15, Ohio

```
comment     Compute the Bessel function I_n (X) when n and X
            are within the bounds of the series expansion.
            The procedure calling statement gives n, X and an
            absolute tolerance δ for determining the point at
            which the terms of the summation become insig-
            nificant. Special case: I_0(0) = 1;
procedure   I(n, X, δ) =: (Is)
begin
I:          s := 0  ;  sum := 0
if          (n ≠ 0)  ;  go to STRT
if          (X = 0)  ;  begin Is := 1  ;  return end
            summ := 1  ;  go to SURE
STRT:       sfac := 1
if          (s = 0)  ;  go to HRE
for         t := 1 (1) s
            sfac := sfac × t
HRE:        snfac := sfac
for         t := s + 1 (1) s + n
            snfac := snfac × t
            summ := sum + (X/2)^(n+2×s)/(sfac × snfac)
SURE: if    (δ < abs (summ − sum))
begin       s := s + 1  ;  sum := summ  ;  go to STRT end
            Is := summ  ;  return
end
```

6. Bessel Function I, Asymptotic Expansion

Dorothea S. Clarke
General Electric Co., FPLD, Cincinnati 15, Ohio

```
comment     Compute the Bessel Function I_n(X) when n and X
            are within the bounds of the asymptotic expansion.
            The procedure calling statement gives n, X and an
            absolute tolerance δ for determining the point at
            which the terms of the summation become in-
            significant;
procedure   I(n, X, δ) =: (IA)
begin
I:          r := 1  ;  pe := (4 × n² − 1) / (8 × X)
              sum := − pe
Repeat:     r := r + 1
            pe := pe × ((2 × n)² − (2 × r − 1)²) / (r × 8 × X)
if          (δ < abs (pe))
begin       sum := sum + (−1)^r × pe  ;  go to Repeat end
            IA := (1 + sum) × (exp(X) / sqrt (2 × π × X))
              return
end
```

7. Euclidian Algorithm

Robert Claussen
General Electric Co., Cincinnati 15, Ohio

```
comment     Every pair of numbers a, b not both zero have a
            positive greatest common divisor: gcd;
procedure   EUC (a, b) =: (gcd)
begin
EUC:
if          (a = 0)
begin       gcd := b   ;  return end
if          (b = 0)
begin       gcd := a   ;  return end
            r2 := a
            r1 := b
here:       g := r2/r1
comment     Assumption is made that truncation takes place
            in the above statement;
            r := r2 − r1 × g
if          (r = 0)
begin       gcd := r1   ;  return end
begin       r2 := r1
            r1 := r
            go to here end
integer     (g)
end
```

ALGORITHM 8
EULER SUMMATION
3 (May 1960), 318 P. NAUR

```
procedure euler (fct, sum, eps, tim) ; value eps, tim ;
integer tim ; real procedure fct ; real sum, eps ;
comment euler computes the sum of fct(i) for i from zero up to
infinity by means of a suitably refined euler transformation. The
summation is stopped as soon as tim times in succession the abso-
lute value of the terms of the transformed series are found to be
less than eps. Hence, one should provide a function fct with one
integer argument, an upper bound eps, and an integer tim. The
output is the sum sum. euler is particularly efficient in the case
of a slowly convergent or divergent alternating series ;
begin integer i, k, n, t ; array m[0:15] ; real mn, mp, ds ;
i := n := t := 0 ; m[0] := fct(0) ; sum := m[0]/2 ;
nextterm: i := i+1 ; mn := fct(i) ;
        for k := 0 step 1 until n do
            begin mp := (mn+m[k])/2 ; m[k] := mn ;
              mn := mp end means ;
        if (abs(mn)<abs(m[n]))∧(n<15) then
            begin ds := mn/2 ; n := n+1 ; m[n] :=
              mn end accept
        else ds := mn ;
        sum := sum + ds ;
        if abs(ds)<eps then t := t+1 else t := 0 ;
        if t<tim then go to nextterm
end euler
```

CERTIFICATION OF ALGORITHM 8
EULER SUMMATION [P. Naur et al. *Comm. ACM* 3, May 1960]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

The body of *euler* was tested on the LGP-30 computer using the Dartmouth SCALP translator. No errors were detected.

The program gave excellent results when used to derive the coefficients for the expansion of $ln\ (1+x)$ in shifted Chebyshev polynomials from the first ten terms of the power series. For $n = 0, 1, 2, 3, 4$, the coefficient of x^i in the power series was multiplied by the coefficient of $T_n^*(x)$ in the expression of x^i in terms of the $T_n^*(x)$. The product, for $i = 1, 2, \cdots, 10$ was used as $fct(i)$ in the program. Results for $n = 0$ were as follows:

i	*fct(i)*	*ds*	*sum*
1	+0.50000000	—	—
2	−0.18750000	+0.07812500	+0.3281250
3	+0.10416667	+0.05729166	+0.3854167
4	−0.068359375	−0.005940758	+0.3794759
5	+0.049218750	−0.001928713	+0.3775471
6	−0.037597656	−0.001357019	+0.3761900
7	+0.029924665	+0.0001742393	+0.3763642
8	−0.024547577	+0.0000571311	+0.3764212
9	+0.020607842	+0.0006395427	+0.3764607
10	−0.017619705	−0.0000055069	+0.3764551
True Value[1]			+0.3764528129.....

Errors less than 0.2×10^{-5} were also found for $n = 1, 2, 3, 4, 5, 6, 7, 8$ and 9.

This technique appears to be a useful supplement to direct telescoping (Algorithms 37 and 38) and to the methods recommended by Clenshaw[1], for slowly convergent power series.

---

[1] Clenshaw, C. W., *Chebyshev Series for Mathematical Functions.* National Physical Laboratory Math Tables, Vol. 5, London, H.M.S.O. (1962).

ALGORITHM 9 RUNGE-KUTTA INTEGRATION
3 (May 1960), 318 P. NAUR

```
procedure RK(x,y,n,FKT,eps,eta,xE,yE,fi) ; value x,y ;
integer n ; Boolean fi ; real x,eps,eta,xE ; array
y,yE ; procedure FKT ;
comment : RK integrates the system y_k'=f_k(x,y_1,y_2,... ,y_n)
(k=1,2,... ,n) of differential equations with the method of Runge-
Kutta with automatic search for appropriate length of integration
step. Parameters are: The initial values x and y[k] for x and the un-
known functions y_k(x). The order n of the system. The procedure
FKT(x,y,n,z) which represents the system to be integrated, i.e.
the set of functions f_k . The tolerance values eps and eta which
govern the accuracy of the numerical integration. The end of the
integration interval xE. The output parameter yE which repre-
sents the solution at x=xE. The Boolean variable fi, which must
always be given the value true for an isolated or first entry into
RK. If however the functions y must be available at several mesh-
points x_0 , x_1 , ... , x_n , then the procedure must be called repeat-
edly (with x=x_k , xE=x_k+1, for k=0, 1, ... , n-1) and then the
later calls may occur with fi=false which saves computing time.
The input parameters of FKT must be x,y,n, the output parameter
z represents the set of derivatives z[k]=f_k(x,y[1], y[2], ... , y[n])
for x and the actual y's. A procedure comp enters as a non-local
identifier ;
begin
  array z,y1,y2,y3[1:n] ; real x1,x2,x3,H ; Boolean out ;
  integer k,j ; own real s,Hs ;
  procedure RK1ST(x,y,h,xe,ye) ; real x,h,xe ; array
          y,ye ;
    comment : RK1ST integrates one single RUNGE-KUTTA
          with initial values x,y[k] which yields the output
          parameters xe=x+h and ye[k], the latter being the
          solution at xe. Important: the parameters n, FKT, z
          enter RK1ST as nonlocal entities ;
    begin
      array w[1:n], a[1:5] ; integer k,j ;
      a[1] := a[2] := a[5] := h/2 ; a[3] := a[4] := h ;
      xe := x ;
      for k := 1 step 1 until n do ye[k] := w[k] := y[k] ;
      for j := 1 step 1 until 4 do
      begin
        FKT(xe,w,n,z) ;
        xe := x+a[j] ;
        for k := 1 step 1 until n do
        begin
          w[k] := y[k]+a[j]×z[k] ;
          ye[k] := ye[k] + a[j+1]×z[k]/3
        end k
      end j
    end RK1ST ;
Begin of program:
    if fi then begin H := xE-x ; s := 0 end else H := Hs ;
    out := false ;
AA: if (x+2.01×H-xE>0)≡(H>0) then
    begin Hs := H ; out := true ; H := (xE-x)/2
      end if ;
    RK1ST (x,y,2×H,x1,y1) ;
BB: RK1ST (x,y,H,x2,y2) ; RK1ST(x2,y2,H,x3,y3) ;
    for k := 1 step 1 until n do
      if comp(y1[k],y3[k],eta)>eps then go to CC ;
    comment : comp(a,b,c) is a function designator, the value
      of which is the absolute value of the difference of the
      mantissae of a and b, after the exponents of these
      quantities have been made equal to the largest of the ex-
      ponents of the originally given parameters a,b,c ;
    x := x3 ; if out then go to DD ;
    for k := 1 step 1 until n do y[k] := y3[k] ;
    if s=5 then begin s := 0 ; H := 2×H end if ;
    s := s+1 ; go to AA ;
CC: H := 0.5×H ; out := false ; x1 := x2 ;
    for k := 1 step 1 until n do y1[k] := y2[k] ;
    go to BB ;
DD: for k := 1 step 1 until n do yE[k] := y3[k]
end RK
```

[8] This RK-program contains some new ideas which are related to ideas of S. GILL, A process for the step-by-step integration of differential equations in an automatic computing machine, *Proc. Camb. Phil. Soc. Vol. 47* (1951) p. 96; and E. FRÖBERG, On the solution of ordinary differential equations with digital computing machines, *Fysiograf. Sällsk. Lund, Förhd. 20* Nr. 11 (1950) p. 136–152. It must be clear, however, that with respect to computing time and round-off errors it may not be optimal, nor has it actually been tested on a computer.

CERTIFICATION OF ALGORITHM 9 [D2] RUNGE-KUTTA INTEGRATION [P. Naur et al., *Comm. ACM 3* (May 1960), 318]

HENRY C. THACHER, JR. (Recd. 28 July 1964 and 22 Nov. 1965)

Argonne National Laboratory, Argonne, Ill.

Algorithm 9 was transcribed into the hardware representation for CDC 3600 ALGOL and run successfully. The following procedure was used for the global procedure *comp*:

```
real procedure comp (a, b, c); value a, b, c; real a, b, c;
begin integer AE, BE, CE;
  integer procedure expon(x); real x;
  comment This function produces the base 10 exponent of x;
  expon := if x = 0 then -999 else
    entier (.4342944819 × ln(abs(x)) + 1);
  comment The number -999 may be replaced by any number
    less than the exponent of the smallest positive number handled
    by the particular machine used, for this algorithm assumes
    that true zero has an exponent smaller than any nonzero
    floating-point number. Users implementing real procedure
    comp by machine code should make sure that this condition
    is satisfied by their program;
  AE := expon(a); BE := expon(b); CE := expon(c);
  if AE < BE then AE := BE; if AE < CE then AE := CE;
  comp := abs(a - b)/10 ↑ AE
end
```

This has the advantage of machine independence, but is highly inefficient compared to machine code.

The procedure was tested using the two following procedures for *FKT*:

```
procedure FKT (X, Y, N, Z); real X; integer N; array Y, Z;
comment (dy1/dx) = z1 = y2, (dy2/dx) = z2 = −y1. With y1(0) = 0, y2(0) = 1, the solution is y1 = sin x, y2 = cos x;
begin Z [1] := Y [2]; Z [2] := −Y [1] end;
procedure FKT (X, Y, N, Z); real X; integer N; array Y, Z;
comment (dy1/dx) = 1 + y1². For y1(0) = 0, y(x) = tan x;
Z [1] := 1+Y[1]↑2;
```

The *RK* procedure was used to integrate the differential equations represented by the first *FKT* procedure from $x = 0(0.5)7.0$, with $eps = eta = 10^{-6}$, and with $y_1(0) = 0$, $y_2(0) = 1$. The actual step size h was .0625 for most of the range, but was reduced to .03125 in the neighborhood of $x = k\pi/2$, where one or the other of the solutions is small.

The computed solutions at $x = 7.0$ were: $y_1 = 6.5698602746 \times 10^{-1}$, $y_2 = 7.5390270246 \times 10^{-1}$, with errors -5.71×10^{-7} and 4.48×10^{-7}, respectively.

Results for the second differential equation are summarized in Table I below.

The efficiency of the procedure would be increased slightly on most computers by changing the type of the **own** variable *s* from **real** to **integer.**

The error is estimated by comparing the results of successive pairs of steps with that of a single double step. This is somewhat more time-consuming than the Kutta-Merson process presented in Algorithm 218 [*Comm. ACM 6* (Dec. 1963) 737-8]. However, the criterion for step-size variation in Algorithm 9 which effectively applies an approximate relative error criterion, *eps*, for $|y| > eta$, and an absolute error criterion $eta \times eps$, for $|y| < eta$, appears superior when the solution fluctuates in magnitude.

TABLE I [ALG. 9]

		$x = 0.5$			$x = 1.0$			$x = 1.5$		
	η	h_{min}	*Absolute error*	*Relative error*	h_{min}	*Absolute error*	*Relative error*	h_{min}	*Absolute error*	*Relative error*
10^{-7}	10^{-3}	.03125	-1×10^{-9}	-2×10^{-9}	.03125	9×10^{-8}	6×10^{-8}	.00390625	-1×10^{-6}	-8×10^{-8}
10^{-5}	10^{-3}	.125	-5×10^{-7}	-9×10^{-7}	.0625	8×10^{-7}	5×10^{-7}	.0078125	-2×10^{-4}	-1×10^{-5}
10^{-3}	10^{-3}	.25	-1×10^{-5}	-2×10^{-5}	.25	-2×10^{-4}	-1×10^{-4}	.03125	-3×10^{-2}	-2×10^{-3}

10. Evaluation of the Chebyshev Polynomial $T_n(X)$ by Recursion

G. M. Galler
National Bureau of Standards, Washington 25, D. C.

```
comment        This procedure computes the Chebyshev
               polynomial Tn(X) = cos (n × cos⁻¹(X)) for
               any given real argument, X, and any order, n,
               by the recursion formula below;
real procedure Ch(n, X) ;
real           X ; integer n ;
begin real     a, b, c ; integer i ;
               a := 1 ; b := X ;
               if n = 0 then c := a else if n = 1 then
               c := b else for i := 2 step 1 until n do
               begin  c := 2 × X × b − a ;
                      a := b ; b := c
               end
               Ch := c
               end
```

CERTIFICATION OF ALGORITHM 10 CHEBYSCHEV POLYNOMIAL $T_n(x)$ (Galler, *Comm. ACM*, June, 1960)

John Herndon
Stanford Research Institute, Menlo Park, California

When transliterated into BALGOL and tested on the Burroughs 220, Ch(n, x) gave better than 7-digit accuracy for n = 0, 1, 4, 8 and x = .01, .2, .7. It gave answers when x > 1 which corresponded to the value of the series with x substituted.

11. EVALUATION OF THE HERMITE POLYNOMIAL $H_n(X)$ BY RECURSION

G. M. Galler
National Bureau of Standards, Washington 25, D. C.

```
comment        This procedure computes the Hermite poly-
               nomial
               Hn(X) = (-1)^n × e^X^2 × (d^n/dX^n(e^-X^2)) for any
               given real argument, X, and any order, n, by
               the recursion formula below;
real procedure He(n, X) ;
integer        n ; real X ;
begin real     a, b, c ; integer i ;
               a := 1 ; b := 2X
               if n = 0 then c := a else if n = 1 then
               c := b else for i := 1 step 1 until n-1 do
               begin  c := 2 × X × b - 2 × i × a ;
                      a := b ; b := c
               end
               He := c
               end
```

12. Evaluation of the Laguerre Polynomial $L_n(X)$ by Recursion

G. M. Galler
National Bureau of Standards, Washington 25 D. C.

```
comment        This procedure computes the Laguerre polynomial
               Ln(X) = e^X × (d^n/dX^n(X^n × e^-X)) for any
               given real argument, X, and any order, n, by
               the recursion formula below;
real procedure La(n, X) ;
integer        n ; real X ;
begin real     a, b, c ; integer i ;
               a := 1 ; b := 1 − X ;
               if n = 0 then c := a else if n = 1 then
               c := b else for i = 1 step 1 until n−1 do
           begin c := (1+2×i−X)×b−(i↑2)×a ;
                 a := b ; b := c
               end
               La := c
               end
```

13. Evaluation of the Legendre Polynomial $P_n(X)$ by Recursion

G. M. Galler
National Bureau of Standards, Washington 25 D. C.

```
comment        This procedure computes the Legendre poly-
               nomial
               Pn(X) = (1/(2^n × n!)) × d^n/dX^n(X^2 − 1)^n for
               any given real argument, X, and any order, n,
               by the recursion formula below;
real procedure Le(n, X) ;
integer        n ; real X ;
begin real     a, b, c ; integer i ;
               a := 1 ; b := X ;
               if n = 0 then c := a else if n = 1 then
               c := b else for i := 1 step 1 until n−1 do
          begin c := b × X + (i/(i + 1)) × (X × b − a) ;
                a := b ; b := c
               end
               Le := c
               end
```

CERTIFICATION OF ALGORITHM 13 LEGENDRE POLYNOMIAL $P_n(x)$ (Galler, *Comm. ACM*, June 1960)

John Herndon
Stanford Research Institute, Menlo Park, California

When transliterated into BALGOL and tested on the Burroughs 220, Le(n, x) gave 7-digit accuracy for n = 0, 1, 4, 9 and X = .01, .2, .7, 1.9, 5.0.

ALGORITHM 14
COMPLEX EXPONENTIAL INTEGRAL

A. Beam
National Bureau of Standards, Washington 25, D. C.

```
procedure   EKZ(x,y,k,ϵ,u,v,n) ; real x,y,k,ϵ,u,v ;
              integer n ;
comment     EKZ computes w(z,k) = u + iv = z^k e^z ∫_z^∞ e^-t dt/t^k
            from the continued fraction representation found
            in H. S. Wall, Continued Fractions, Chap. 18 (D.
            Van Nostrand, New York, 1948). Input parameters
            are x, y, k, and ϵ where z=x+iy. Successive con-
            vergents are computed as follows: For n = 2, 3, 4,
            ···, D_n = z/(z + M × D_n-1), R_n =
            (D_n − 1)R_n-1 , C_n = C_n-1 + R_n , where M is
            k + (n−2)/2 or (n−1)/2 according to whether n
            is even or odd, and D_1 = R_1 = C_1 = 1. Computa-
            tion is stopped when C_n and C_n-1 agree to the sig-
            nificance specified by ϵ. The corresponding index
            n is available after use of the procedure. This
            method is valid in the entire complex plane except
            for the origin and the negative real axis. Conver-
            gence is too slow to be practical for | z | < .05.
            Also for some range within the half-strip | y | < 2,
            x < 0 (this range depends on k). The method is
            valid for complex k, but only real k is considered
            in this procedure;
begin       real t1, t2, t3, M, K, c, a, d, b, g, h, ϵ1 ;
              integer m ;
            comment R = a + ib, D = c + id, C = g + ih ;
              ϵ1 := ϵ↑2 ;
            u := c := a := 1 ; v := d := b := 0 ;
              n := 1 ; K := k − 1 ;
BACK:       g := u ; h := v ; n := n + 1 ;
              m := n ÷ 2 ,
            if 2 × m = n then M := m + K else M := m ;
            t1 := x + M × c ; t2 := y + M × d ;
              t3 := t1↑2 + t2↑2 ;
            c := (x × t1 + y × t2)/t3 ;
              d := (y × t1 − x × t2)/t3 ;
            t1 := c − 1 ; t2 := a ;
              a := a × t1 − d × b ; b := d × t2 + t1 × b ;
            u := g + a ; v := h + b ;
            if (a↑2 + b↑2)/(u↑2 + v↑2) > ϵ1 then go to
              BACK ;
end         EKZ
```

CERTIFICATION OF ALGORITHM 14
COMPLEX EXPONENTIAL INTEGRAL (A. Beam, *Comm. ACM*, July, 1960)

P. J. Rader and Henry C. Thacher, Jr.*
Argonne National Laboratory, Argonne, Illinois

EKZ was programmed by hand for the Royal-Precision LGP-30 computer, using a 28-bit mantissa floating-point interpretive system (24.2 modified). To facilitate comparison with existing tables (National Bureau of Standards Applied Mathematics Series 51 and 37), the real and imaginary parts of $E_k(z)$ were computed from u and v. Results are shown in the following table. In all cases, the values agreed with tabulated values within the tolerance specified.

x	y	k	ϵ	n
1×10^{-8}	1.0	1	10^{-1}	7
1×10^{-8}	1.0	1	10^{-2}	14
1×10^{-8}	1.0	1	10^{-3}	24
1×10^{-8}	1.0	1	10^{-4}	37
1×10^{-8}	1.0	1	10^{-5}	52
1×10^{-8}	1.0	1	10^{-6}	70
1×10^{-8}	1.0	1	10^{-7}	90
1×10^{-8}	1.0	1	10^{-8}	114
1×10^{-8}	2.0	1	10^{-6}	37
1×10^{-8}	3.0	1	10^{-6}	26
1×10^{-8}	4.0	1	10^{-6}	21
1.0	1×10^{-8}	1	10^{-6}	40
1.0	1.0	1	10^{-6}	34
1.0	2.0	1	10^{-6}	26
1.0	3.0	1	10^{-6}	21
2·0	1×10^{-8}	1	10^{-6}	23
2.0	1.0	1	10^{-6}	22
2.0	2.0	1	10^{-6}	20
2.0	3.0	1	10^{-6}	17
3.0	1×10^{-8}	1	10^{-6}	17
3.0	1.0	1	10^{-6}	17
3.0	2.0	1	10^{-6}	16
3.0	3.0	1	10^{-6}	15
4.0	0.0	0	10^{-6}	20
4.0	0.0	1	10^{-6}	15
4.0	0.0	2	10^{-6}	16
4.0	0.0	3(1)14	10^{-6}	17
4.0	0.0	15, 16	10^{-6}	16

It thus appears that the algorithm gives satisfactory accuracy, but that in certain ranges of the variables, the time required may be excessive for extensive use.

ALGORITHM 15

ROOTFINDER II (Modification of Algorithm 2. ROOTFINDER, J. Wegstein, *Communications ACM*, February, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

```
procedure   ROOT II (f, a, eps, n, g, c, m); integer n, m;
              real procedure f; real a, eps, g, c;
comment     ROOT II computes a value of g = y satisfying
              the equation y = f(y). The iteration will con-
              verge to Y providing that at some time in the
              iteration a g is reached such that abs(g − Y) ×
              abs(d(df/dy)/dy) < 2 × abs((df/dy) − 1),
              where the derivatives are evaluated at Y.
              Input includes (1) f, a procedure for computing
              f(y), (2) a, an initial approximation to the
              root, (3) eps, a tolerance for the relative error
              in g, and (4) n, a maximum number of itera-
              tions to be performed. Output includes: (1) g,
              the required root, (2) c = f(g) − g, (3) m, a
              parameter indicating the success of the pro-
              cedure. If the tolerance was not met, m < 0.
              | m − 1 | gives the number of times that the
              correction to g exceeded the preceding one, an
              indication of instability. ;
begin integer j; real b, d, h;
            m := 1; if f(0) = 0 then begin g := 0;
              go to return end
            else g := f(a); b := d := c := a − g;
            if c = 0 then go to return else
            for j := 1 step 1 until n do begin c := f(g) − g;
            if (abs(c/g) < eps then go to return else h :=
              b/c;
            if h < 0 ∨ h > 2 then m := m + 1 else
            d := d/(h − 1); b := c; g := g + d end
              iteration
comment     if the system is known to be stable, the if clause
              of the last statement can be omitted;
            m := − m return end
```

* Work supported by the U. S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 15

ROOTFINDER II (Revision by Henry C. Thacher, Jr., *Communications ACM*, August, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

The revision of ROOTFINDER suggested in the preceding remark was programmed by hand for the Royal Precision LGP-30 computer, using a 28-bit mantissa floating point interpretive system (24.2).

The program was tested for the following equations:

(1.k) $f(y) = \arctan y + k\pi$ $(k = 0, 1, 2, 3, 4, 6, 8)$

(2) $f(y) = (y^3 + 1)^{1/3}$

(3) $f(y) = y^3 - 1$

} These both have the root 1.3247180428

(4.k) $f(y) = \sinh \alpha_k y$

(5.k) $f(y) = \cosh \alpha_k y$

} $(\alpha_1 = -1.2,\ \alpha_2 = -0.5,\ \alpha_3 = 0.5,\ \alpha_4 = 1.2)$

Typical results of these tests were as follows.

f(y)	ϵ	a	g	$[f(g_{-1}) - g_{-1}] \times 10^7$	Remarks
1.0	10^{-8}	1.0000	0.0000000	0.00	
1.1	10^{-8}	3.1415	4.4934094	0.15	
1.2	10^{-8}	6.2832	7.7252518	0.60	
1.3	10^{-8}	9.4248	10.904122	0.00	
1.4	10^{-8}	12.5664	14.066194	0.00	
1.6	10^{-8}	18.8496	20.371303	0.60	
1.8	10^{-8}	25.1327	26.666054	0.60	
1.2	10^{-8}	1.3	1.3247179	0.00	
1.2	10^{-8}	0.5	1.3247179	0.00	
3	10^{-9}	9.0	4.4804900	197.74×10^7	Diverged 2 times, not converged after 20 iter.
3	10^{-9}	5.0	1.3482797	$.51 \times 10^7$	
3	10^{-9}	3.0	1.3247180	0.0	Converged in less than 20 iter.
3	10^{-9}	2.0			Diverged 2 times. Term. with h = 1.
3	10^{-9}	1.1	1.3247180	1384.24	Diverged 9 times. Converged after 20 iter.
3	10^{-9}	1.0			Terminated when g became 0.
3	10^{-9}	0.8	1.3247180	0.00	Diverged 4 times. Conv. in less than 20.
3	10^{-9}	0.6	1.6161598	4.39×10^7	Diverged 2 times. No conv. after 20.
4.k	10^{-9}	1.0	0.00000000	0.0000000	For all k.
5.1, 5.4	10^{-8}	1.0	0.09179585	0.793×10^7	Diverged 7 times. No conv. after 20 iter.
5.2, 5.3	10^{-8}	1.0	1.11787755	0.037	

Function (3) is of particular interest, since it does not converge for most algorithms. With the Wegstein iteration, convergence was obtained, or would have been obtained with a few more iterations for a wide range of initial guesses.

* Work supported by the U. S. Atomic Energy Commission.

REMARK ON ALGORITHM 15

ROOTFINDER II (Henry C. Thacher, Jr., *Comm. ACM*, August 1960)

GEORGE E. FORSYTHE AND JOHN G. HERRIOT, Stanford University, Stanford, California

As pointed out by Lieberstein (*Comm. ACM*, January 1959, p. 5), this algorithm is precisely the Newton method of chords or the scant method applied to g(x) = f(x) — x = 0. Thus convergence is not of second order but rather (for simple roots) of order $\frac{1}{2}(\sqrt{5} - 1) = 1.618$, as shown by Jeeves (*Comm. ACM*, August 1958, pp. 9–10). In the first portion of the algorithm b, c, d, should be set equal to g— a instead of a— g in order to be consistent with the iteration portion. Doing this will usually cut down the number of iterations. Not only is a preliminary test for a zero root desirable but the possibility that g may be zero at any stage of the iteration should be considered in writing the return criterion. The possibility that h = 1 should also be checked and appropriate action taken. Algorithm 26 takes care of these matters and also corrects some minor errors in Algorithm 15. This method is certainly not the best rootfinder that could be written.

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

J. H. WILKINSON
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Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the *method* of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \cdots = a_5 = 0$, $a_6 = a_7 = \cdots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^5(x-1)^5(x-2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-44}. Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic. This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, *is a very well-conditioned method of evaluation*. Knowing this, I was able to set a tolerance of 2^{-42} with confidence. If the *same function* had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $|x_{r+1} - x_r|$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$x = n\pi + y$$

$$\tan x - x = -n\pi + \frac{\frac{y^3}{3} - \frac{y^5}{30} - \cdots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^{80} - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable number of iterations are needed to find the root $x = 1$. Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is useful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4, that abs(fprt) < abs(x2 × 10), but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on the size of the function and on the size of the remainders r1 and r0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (Comm. ACM June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to *slow* convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root $x = -6.35099\ 36103$ and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

[1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150–180.

ALGORITHM 16
CROUT WITH PIVOTING
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```
real procedure INNERPRODUCT(u,v) index : (k) start : (s)
                finish : (f);
    value s, f; integer k, s, f; real u, v;
comment         INNERPRODUCT forms the sum of u(k) ×
                v(k) for k = s, s+1, . . . , f. If s > f, the value
                of INNERPRODUCT is zero. The substitution
                of a very accurate inner product procedure
                would make CROUT more accurate;
begin
    real h;
    h := 0; for k := s step 1 until f do h := h + u × v;
    INNERPRODUCT := h
end INNERPRODUCT;

procedure       CROUT (A, b, n, y, pivot, INNERPRODUCT);
    value n; array A, b, y, pivot; integer n, pivot;
    real procedure INNERPRODUCT;
comment         This is Crout's method with row interchanges, as
                formulated in reference [1], for solving Ay = b
                and transforming the augmented matrix [A b]
                into its triangular decomposition LU with all
                L[k, k] = 1. If A is singular we exit to 'singular,'
                a non-local label. pivot[k] becomes the current
                row index of the pivot element in the k-th
                column. Thus enough information is preserved
                for the procedure SOLVE to process a new
                right-hand side without repeating CROUT.
                The accuracy obtainable from CROUT would
                be much increased by calling CROUT with a
                more accurate inner product procedure than
                INNERPRODUCT;
begin
    integer k, i, j, imax, p; real TEMP, quot;
    for k := 1 step 1 until n do
1:  begin
        TEMP := 0;
        for i := k step 1 until n do
2:      begin
            A[i, k] := A[i, k] - INNERPRODUCT(A[i,p], A[p, k],
              p, 1, k-1);
            if abs(A[i, k]) > TEMP then
3:          begin
              TEMP := abs(A[i, k]); imax := i
              end 3
        end 2;
        pivot[k] := imax;
        comment We have found that A[imax, k] is the largest
          pivot in column k. Now we interchange rows k and imax;
        if imax ≠ k then
4:      begin for j := 1 step 1 until n do
5:        begin
          TEMP := A[k,j]; A[k, j] := A[imax,j];
            A[imax,j] := TEMP
          end 5;
          TEMP := b[k]; b[k] := b[imax]; b[imax] := TEMP
        end 4;
        comment The row interchange is done. We proceed to the
                  elimination;
            if A[k, k] = 0 then go to singular;
            for i := k+1 step 1 until n do
            begin quot := 1.0/A[k, k]; A[i, k] := quot × A[i, k]
              end;
            for j := k+1 step 1 until n do
                A[k, j] := A[k,j] - INNERPRODUCT(A[k, p],
                  A[p,j], p, 1, k-1);
                b[k] := b[k] - INNERPRODUCT(A[k,p], b[p], p,
                  1, k-1)
        end 1;
    comment The triangular decomposition is now finished,
              and we do the back substitution;
    for k := n step -1 until 1 do
        y[k] := (b[k] - INNERPRODUCT(A[k,p], y[p], p,
          k+1, n)/A[k, k]
end CROUT;

procedure SOLVE (B, c, n, z, pivot, INNERPRODUCT);
    value n; array B, c, z, pivot; integer n, pivot;
    real procedure INNERPRODUCT;
comment SOLVE assumes that a matrix A has already been
            transformed into B by CROUT, but that a new
            column c has not been processed. SOLVE solves the
            system Az = c, and the output z of SOLVE is pre-
            cisely the same as the output y of the procedure
            statement CROUT (A, c, n, y, pivot, INNER-
            PRODUCT). However, SOLVE is faster, because
            it does not repeat the triangularization of A;
begin
    integer k; real TEMP;
    for k := 1 step 1 until n do
    begin
        TEMP := c[pivot[k]]; c[pivot[k]] := c[k]; c[k] :=
          TEMP; c[k] := c[k] - INNERPRODUCT(B[k, p],
          c[p], p 1, k - 1)
    end;
    for k := n step -1 until 1 do
        z[k] := (c[k] - INNERPRODUCT(B[k,p], z[p], p,
          k+1, n)/B[k, k]
end SOLVE
```

REFERENCE

[1] J. H. WILKINSON, theory and practice in linear systems, pp. 43–100 of JOHN W. CARR III (editor), *Application of Advanced Numerical Analysis to Digital Computers*, (Lectures given at the University of Michigan, Summer 1958, College of Engineering, Engineering Summer Conferences, Ann Arbor, Michigan [1959]).

REMARK ON ALGORITHM 16
CROUT WITH PIVOTING (G. Forsythe, *Communications* ACM, September, 1960)

GEORGE E. FORSYTHE
Stanford University, Stanford, California

QUERY

Perhaps the most basic procedure for an ALGOL library of matrix programs is an inner product procedure. The procedure Innerproduct given on page 311 of [1] is fairly difficult to comprehend, and probably poses great difficulties for most translating routines. I merely copied its form in writing a modified inner product routine for [2].

My query is: How *should* one write an inner product procedure in ALGOL?

REFERENCES

1. PETER NAUR (editor), J. W. BACKUS, ET AL., Report on the algorithmic language ALGOL 60, *Comm. Assoc. Comp. Mach. 3* (1960), 299–314.
2. GEORGE E. FORSYTHE, CROUT with pivoting in ALGOL 60, *Comm. Assoc. Comp. Mach. 3* (1960), 507–508.

REMARK ON ALGORITHM 16
CROUT WITH PIVOTING (G. E. Forsythe, *Comm. ACM, 3* (Sept. 1960), 507–8.)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

This procedure contains the following errors:

a. In SOLVE, the expression

```
c[k] := c[k] − INNERPRODUCT
  (B[k, p], c[p], p  1, k − 1)
```

should read:

```
c[k] := c[k] − INNERPRODUCT
  (B[k, p], c[p], p, 1, k − 1)
```

b. In CROUT, the specification part should read:

```
array A, b, y  ; integer n  ; integer array pivot  ;
```

c. In SOLVE, the specification part should read:

```
array B, c, z  ; integer n  ; integer array pivot  ;
```

The efficiency of the algorithm will be improved by the following changes:

a. In the elimination phase of CROUT, replace

```
for i := k + 1 step 1 until n do
begin quote := 1.0/A[k, k]  ;  A[i, k] := quot XA[i, k] end  ;
```

by

```
quot := 1.0/A[k, k]  ; for i := k + 1 step 1 until n do
    A[i, k] := quot XA[i, k]  ;
```

b. Omit INNERPRODUCT from the formal parameter list in both CROUT and SOLVE, and declare INNERPRODUCT either locally, or globally. This avoids any reference to INNERPRODUCT in the calling sequence produced by a compiler.

It is also to be noted that a minor modification of CROUT allows it to be used to evaluate the determinant of A.

All of these suggestions are included in a later algorithm.

* Work supported by the U. S. Atomic Energy Commission.

ALGORITHM 17
TRDIAG
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```
procedure   trdiag (a,b,c,d) order : (n) result : (x);
value n;    array a, b, c, d, x; integer n;
comment     this procedure gives the solution to the tri-
              diagonal system of linear algebraic equations:
            a1x2 + b1x1 + d1 = 0
            aixi+1 + bixi + cixi-1 + di = 0, i = 2,3, ··· , n-1
            bnxn + cnxn-1 + dn = 0.
            This method is often used to obtain solutions to
              second order difference equations;
begin array gamma [1 : n-1]; integer i; real y;
              gamma [1] := -a[1]/b[1];
            x[1] := -d[1]/b[1];
for         i := 2 step 1 until n-1 do
begin       y = b[i] + c[i] × gamma [i - 1];
            gamma [i] := -a[i]/y; x[i] := -(c[i] × x[i-1]
              + d[i])/y end;
            x[n] := -(c[n] × x[n-1] + d[n])/(b[n] + c[n]
              × gamma [n-1]);
for         i := n step -1 until 2 do
            x[i - 1] := x[i] × gamma [i - 1] + x[i - 1]
end trdiag
```

ALGORITHM 18
RATIONAL INTERPOLATION BY CONTINUED FRACTIONS

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```
comment  This procedure fits to m given points (x_i , y_i) a continued fraction in the form
    a_1+(x-x_1)/(a_2+(x-x_2)/(a_3+(x-x_3)/···(x-x_{m-1})/a_m))···))
    It also simplifies the continued fraction to a rational function
    (N_0+N_1x+···+N_{deg}x^{deg})/(D_0+D_1x+···+D_{deg}x^{deg}),
    where deg is at most m ÷ 2;
procedure  confr(m,x,y,a,N,D);
real array  x,y,a,N,D;  integer m;
begin real  aa, xx, T;  integer i, j, k;  real array P,Q[0 : m ÷ 2
    switch sw := sw1, sw2;
    for j := 1 step 1 until m do
    begin aa := y[j];  xx := x[j];
        for i := 1 step 1 until j-1 do
        aa  := (xx-x[i])/(aa-a[i]);  a[j]  :=  aa
    end;
    k := 1;  P[0] := 1;  Q[0] := a[1];
    mult : for j := 1 step 1 until m ÷ 2 do P[j] := Q[j] := 0;
    for i := 2 step 1 until m do
    begin for j := i ÷ 2 step -1 until 1 do
        begin T := a[i] × Q[j] - x[i-1] × P[j] + P[j-1];
            P[j] := Q[j]; Q[j] := T
        end;  T := a[i] × Q[0] - x[i-1] × P[0];
        P[0] := Q[0];  Q[0] := T
    end;  go  to  sw[k];
    sw1 : for j := 0 step 1 until m ÷ 2 do N[j] := Q[j];
        k := 2;  P[0] := 0; Q[0] := 1;  go to mult;
    sw2 : for j := 0 step 1 until m ÷ 2 do D[j] := Q[j]
end  procedure
```

CERTIFICATION OF ALGORITHM 18
RATIONAL INTERPOLATION BY CONTINUED FRACTIONS

[R. W. Floyd, *Comm. ACM.*, Sept. 1960]

HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

The body of procedure *confr* was tested with the ALGOL translator system written for the LGP-30 computer by the Dartmouth College Computer Center. No syntactical errors were found in the procedure body, except for a missing semicolon after the array delcaration. The translated algorithm gave satisfactory results when tested on values of $(4x + 1)/(x + 4)$ at any three of the points $x = 1, 2, 3, 4$. When all four points were used, a division overflow occurred in the statement **for** i := 1 **step** 1 **until** $j-1$ **do** aa := $(xx - x[i])/(aa-a[i])$; which forms the reciprocal differences. An overflow of this type will occur whenever $y[j]$ is approximated to high accuracy by one of the continued fractions based only on the points $x[i]$, $i = 1, 2, \cdots, k$ with k less than j. Unless $i = j-1$, the difficulty may be overcome by setting aa equal to the largest real representable in the computer whenever division overflow would occur. When $i = j-1$, the difficulty is irretrievable, and the data points must be reordered.

ALGORITHM 19
BINOMIAL COEFFICIENTS

RICHARD R. KENYON
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```
comment          This procedure computes binomial coefficients C_m^n = n!/m!(n — m)! by the recursion formula C_{i+1}^n = (n — 1)C_i^n/(i + 1) starting from C_0^n = 1 ;
integer procedure C(m, n) ;
integer          m, n ;
begin            integer i, a, b ;
                 a := 1 ;
                 if 2 × m > n then b := n — m else
                   b := m ;
                 for i := 0 step 1 until b do
                 begin a := (n — i) × a ÷ (i + 1) end
                 C := a
end              Binomial Coefficients
```

REMARK ON ALGORITHM 19
RINOMIAL COEFFICIENTS (Richard R. Kenyon, *Comm. ACM*, Oct. 1960)

BICHARD STECK
Armour Research Foundation, Chicago 16, Ill.

The **for** clause of Algorithm 19 should read:

for i := 0 **step** 1 **until** b−1 **do**

With this correction the algorithm was certified on the Armour Research Foundation UNIVAC 1105.

The recursion formula stated in the **comment** should read:

$$C_{i+1}^n = (n-i)\ C_i^n/(i+1).$$

CERTIFICATION OF ALGORITHM 19
BINOMIAL COEFFICIENTS [Richard R. Kenyon, *Comm. ACM* Oct., 1960]

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* Work supported by the U. S. Atomic Energy Commission.

This procedure was tested on the LGP-30, using the compiler ALGOL-30 from Dartmouth College Computation Center. The following changes were found necessary:

(1) Within the **comment**, the line

$$C_{i+1}^n = (n - 1)C_i^n/(i + 1)$$

should be

$$C_{i+1}^n = (n - i)C_i^n/(i + 1)$$

(2) The line defining the iteration loop

for *i* := 0 **step** 1 **until** *b* **do**

should be

for *i* := 0 **step** 1 **until** *b*−1 **do**

(3) The sequence

end *C* := *a* **end**

should be

end; *C* := *a* **end**

ALGORITHM 20
REAL EXPONENTIAL INTEGRAL

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```
real procedure   Expint (x) ; real x ;
comment          -Ei(-x) = ∫_x^∞ (e^-u/u) du is computed for
                 x > 0 by approximation formulas. For
                 0 < x < 1 the approximation is from E. E.
                 Allen, Note 169, MTAC 56, pg 240 (1954).
                 The second approximation formula is for
                 1 ≤ x < ∞ and is from C. Hastings, Jr.,
                 "Approximations For Digital Computers"
                 (Princeton University Press, Princeton,
                 New Jersey, 1955). The absolute error
                 ε(x) is |ε(x)| < 2 × 10^-7 for 0 < x < 1
                 and |ε(x)| < 2 × 10^-8 for 1 ≤ x < ∞ ;
begin            real y, w, z ;
                 if x < 1 then
                 z := (((( .00107857 × x — .00976004) × x
                   + .005519968) × x — .24991055) × x
                   + .99999193) × x — .57721566 — ln(x)
                 else begin
                 y := ((( x + 8.5733287401) × x
                   + 18.059016973) × x + 8.6347608925) × x
                   + .2677737343 ;
                 w := ((( x + 9.5733223454) × x
                   + 25.6329561486) × x
                   + 21.0996530827) × x + 3.9584969228 ;
                 z := exp (—x) /x × (y/w) end
                 Expint := z end
```

REMARK ON ALGORITHM 20
REAL EXPONENTIAL INTEGRAL (S. Peavy, *Comm. ACM*, October 1960)

S. PEAVY
National Bureau of Standards, Washington, D. C.

A printing error has been called to our attention by J. A. Beutler of E. I. duPont de Nemours and Co. Lines 15 through 17 of Algorithm 20 should read

```
z := (((.00107857 × x − .00976004) × x
  + .05519968) × x − .24991055) × x
  + .99999193) × x − .57721566 − ln (x)
```

* Work supported by the U. S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 20
REAL EXPONENTIAL INTEGRAL (S. Peavy, *Comm. ACM*, Oct. 1960)

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Expint (x) was programmed for the LGP-30 computer, using both a 7S floating-point compiler (ACT III) and an 8S floating-point interpretive code (24.2). Constants given to more than 7S (or to 8S for the 24.2 program) were rounded to 7S (or 8S).

After changing the constant .005519968 to .05519968, both programs gave acceptable accuracy over the range tested.

The 8S (24.2) program was compared with the 9D values given for $-E_i(-x)$ in Mathematical Tables Project, *Tables of Sine, Cosine, and Exponential Integrals, Volume* II (1940) for the set of values x = 0.1(0.1)1.0(1.0)10.0. The largest discrepancy found was -16×10^{-8} for x = 0.1. For x greater than 1, all values tested were good to 8S.

For computing real values of the exponential integral, this algorithm is much faster than EKZ (Algorithm 13). For x < 1, the ratio of speeds was of the order of 20.

* Work supported by the U.S. Atomic Energy Commission.

ALGORITHM 21

BESSEL FUNCTION FOR A SET OF INTEGER ORDERS

W. BÖRSCH-SUPAN

National Bureau of Standards, Washington 25, D. C.

```
procedure BESSELSETINT (x, n, ϵ, J) ; value x, n, ϵ ;
    real x, ϵ ; integer n ; real array J ;
comment: This procedure computes the values of the Bessel
    functions Jp(x) for real argument x and the set of all integer
    orders from 0 up to n and stores these values into the array J,
    whose subscript bounds should include the integers from 0 up
    to n. n must be nonnegative.
      The computation is done by applying the recursion formula
    backward from p = k down to p = 0 as described in MTAC 11
    (1957), 255-257. k is chosen to yield errors less than 10^-5
    approximately after the first application of the recursion. The
    recursion is repeated with a larger k until the difference be-
    tween the results of the two last recursions doesn't exceed the
    given bound ϵ > 0. The steps in increasing k are chosen in
    such a way that the errors decrease at least by a factor of
    approximately 10^-5. There is no protection against overflow. ;
begin real dist, rec0, rec1, rec2, sum, max, err ;
    integer k, p ; Boolean s ; real array Jbar[0:n] ;
    if x = 0 then
    begin J[0] := 1 ; for p := 1 step 1 until n do J[p] := 0 ;
      go to Exit
    end ;
    dist := if abs(x) ≧ 8 then 5 × abs(x) ↑ (1/3) else 10 ;
    k := entier ((if abs(x) ≧ n then abs(x) else n) + dist) + 1 ;
    s := false ;
Rec: rec0 := 0 ; rec1 := 1 ; sum := 0 ;
    for p := k step -1 until 1 do
    begin J[if p > n + 1 then n else p - 1] := rec2 :=
            2 × p/x × rec1 - rec0 ;
          if p = 1 then sum := sum + rec2
          else if p ÷ 2 × 2 ≠ p then sum :=
            sum + 2 × rec2 ;
          rec0 := rec1 ; rec1 := rec2
    end   recursion ;
Norm: for p := 0 step 1 until n do J[p] := J[p]/sum ;
    if s then
    begin max := 0 ;
          for p := 0 step 1 until n do
          begin err := abs (J[p] - Jbar[p]) ;
                if err > max then max := err
          end   maximum error ;
          if max ≦ ϵ then go to Exit
    end then
    else s := true ;
    for p := 0 step 1 until n do Jbar[p] := J[p] ;
    k := entier (k + dist) ;
    go to Rec ;
Exit: end BESSELSETINT
```

CERTIFICATION OF ALGORITHM 21 [S17]

BESSEL FUNCTION FOR A SET OF INTEGER ORDERS

[W. Börsch-Supan, *Comm. ACM 3* (Nov. 1960), 600]

J. STAFFORD (Recd. 16 Nov. 1964)

Westland Aircraft Ltd., Saunders-Roe Division, East Cowes, Isle of Wight, Eng.

If this procedure is used with a combination of a moderately small argument and a moderately large order, the recursive evaluation of *rec2* in the last line of the first column can easily lead to overflow. This occurred, for instance, in trying to evaluate $J_{10}(0.01)$.

The following alterations correct this:

(i) Declare a **real** variable z and an **integer** variable m;

(ii) After line *rec* insert:

```
z := MAX/4 × abs (x/k);
comment MAX is a large positive number approaching in
    size the largest number which can be represented. The nu-
    merical value of MAX/4 is written into the procedure;
```

(iii) At the end of the first column insert:

```
if abs(rec2) > z then
begin
    rec1 := rec1/z; rec2 := rec2/z; sum := sum/z;
    for m := n step -1 until p - 1 do J[m] := J[m]/z
end;
```

With these alterations the procedure was run on a National-Elliott 803, for $x = -1, 0, 0.01, 1, 10$ and $n = 0, 1, 2, 10, 20$. The results agreed exactly with published seven-place tables.

[See also Algorithm 236, Bessel Functions of the First Kind (*Comm. ACM 7* (Aug. 1964), 479) which is not restricted to integer values. Although it is a much more complicated program, Algorithm 236 is slightly faster than Algorithm 21 as corrected, at least in some cases.—Ed.]

ALGORITHM 22
RICCATI-BESSEL FUNCTIONS OF FIRST AND SECOND KIND
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```
procedure RICCATIBESSEL (x, n, eps, S, C) ;
    value x, n, eps ;
    real x, eps; integer n; real array S, C ;
comment: RICCATIBESSEL computes S_k(x) = (πx/2)^½ J_{k+½}(x)
    and C_k(x) = −(πx/2)^½ Y_{k+½}(x) for real x ≠ 0 and all integer
    values of k from 0 through n with a prescribed (absolute)
    accuracy eps. The computation is done by using the recursion
    relations of the cylinder functions. For abs(x) > n both S_k(x)
    and C_k(x) are computed by using the recursions for ascending
    orders. For n > abs(x) the functions S_k(x) are obtained by
    using the recursion in descending orders. (See STEGUN-
    ABRAMOWITZ, MTAC 11, 1957, 255-257). Reaching out two
    different intervals beyond the order n, the two vectors S_k^1(x)
    and S_k^2(x) are checked if the maximum component of their
    difference meets the tolerance eps. If this is not the case a
    maximum of 10 iterations is set up to achieve the required
    absolute accuracy. Initial values S_kmax and S_kmax−1 for the
    backward iteration are computed from the corresponding
    values C_kmax−1 and C_kmax. No check of accuracy is done in
    case n < abs(x). Both C_k(x) and S_k(x) are affected in this
    case by errors of the same order of magnitude as the sub-
    routines for sin (x) and cos (x) ;
begin real r1, r2, r3, r4, r5, r6, step, acc, max, a, b, d1, d2 ;
    integer i, k, l, imax ;
    real array W[o:n] ;
    switch P := initial, improve ;
    acc: = 10^-6 ;
    step: = 10^3 ;
    imax: = 10 ;
    comment: These constants may be chosen differently, but
        caution has to be taken because of overflow. acc sets an
        initial iteration to give roughly a 6-place accuracy.
        Subsequent iterations should improve the result to 3 more
        places each ;
    i := 1 ;
    if x = 0 then go to exit1 ;
    if n < abs(x) then
case1: begin r1 := −sin(x) ; r2 := r4 := C[0] := cos(x) ;
            r5 := S[0] := sin(x) ;
            for k := 1 step 1 until n do
            begin C[k] := r3 := (2×k−1) × r2/x − r1 ;
                  S[k] := r6 := (2×k−1) × r5/x − r4 ;
                  r1 := r2 ; r2 := r3 ;
                  r4 := r5 ; r5 := r6
            end k ; go to finish
       end case1 ;
case2: l := 1 ; r1 := −sin(x) ; r2 := C[0] := cos(x) ;
       for k := 1 step 1 until n do
       begin C[k] := r3 := (2×k−1) × r2/x − r1 ;
             r1 := r2 ;
             r2 := r3
       end ;
       a := n ;
loop:  for k := 1+n step 1 until if abs(x) ≦ 11
         then 12+a else 2×a+1 do
       begin r3 := (2×k−1) × r2/x − r1 ;
             if abs(r3/C[n]) > acc then go to S ;
             r1 := r2 ;
             r2 := r3 ;
             comment: This loop is most liable to cause
                      overflow ;
       end loop ;
       k := if abs(x) ≦ 11 then 12+a else 2×a + 1 ;
       r2 := r1 ;
S:     r6 := x ↑ 2/(4×k ↑ 2×r2) ;
       r5 := 1/r3 ;
       go to P[l] ;
initial: for k := k step −1 until 2 do
       begin W[if k>n+2 then n else k−2] := r4 :=
               (2×k−1) × r5/x − r6 ;
             r6 := r5 ;
             r5 := r4
       end ;
       d1 := r5/x − r6 ;
       d2 := if abs(W[0]) ≧
         abs(d1) then sin(x)/W[0] else cos(x)/d1 ;
       for k := 0 step 1 until n do
           W[k] := d2×W[k] ;
       acc := step × acc ;
       l := 2 ;
       a := a + step ↑ (1/3) ;
       r2 := C[n] ;
       r1 := C[n—1] ;
       go to loop ;
improve: for k := k step —1 until 2 do
       begin S[if k > n+2 then n else k−2] := r4 :=
               (2×k−1) × r5/x−r6 ;
             r6 := r5 ;
             r5 := r4
       end k ;
       d1 := r5/x − r6 ;
       d2 := if abs(S[0]) ≧
         abs(d1) then sin(x)/S[0] else cos(x)/d1 ;
       max := 0 ;
       for k := 1 step 1 until n do
       begin S[k] := d2×S[k] ;
             b := abs(S[k] − W[k]) ;
             if b > max then max := b
       end ;
       if max < eps then go to finish ;
       for k := 0 step 1 until n do W[k] := S[k] ;
           acc := step × acc ;
           if i ≧ imax then go to exit2 ;
           i := i+1 ; a := a + step ↑ (1/3) ;
           r2 := C[n] ; r1 := C[n—1] ; go to loop ;
exit1: go to finish ; comment: x = 0 ;
exit2: go to finish ;
       comment: maximum number of iterations reached ;
finish: end RICCATIBESSEL
```

CERTIFICATION OF ALGORITHM 22 [S17] RICATTI-BESSEL FUNCTIONS OF FIRST AND SECOND KIND [H. Oser, *Comm. ACM 3* (Nov. 1960), 600]

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KEY WORDS AND PHRASES: Ricatti-Bessel functions, Bessel functions of fractional order, spherical Bessel functions
CR CATEGORIES: 5.12

The procedure was translated into FORTRAN IV and run on an IBM 360/44 using double precision arithmetic (15 significant decimal digits). One error was discovered in the algorithm. The tenth line following the line with the label "*improve*" reads:

for k := 1 **step** 1 **until** n **do**

This line should read:

for k := 0 **step** 1 **until** n **do**

The results $S_k(x)/x$ and $-C_k(x)/x$ were computed using this correction and compared with Tables 10.1, 10.2 and 10.5 of [1]. The results agreed to the number of digits given in the tables for:

x	k
0.1	0(1)8
0.5	0(1)8
1.0	0(1)20
2.0	0(1)8
5.0	0(1)50
7.5	0(1)8
10.0	0(1)50
50.0	0(1)100
100.0	0(1)100

REFERENCES:

1. ABRAMOWITZ, M., AND STEGUN, I. A. *Handbook of Mathematical Functions*. Appl. Math. Ser. 55, Nat. Bur. Standards US Govt. Print. Off., Washington, D.C., 1964.

ALGORITHM 23
MATH SORT
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```
procedure MATHSORT (INVEC, OUTVEC, TOTEVEC,
    n, k, SETFUNC) ; value n, k ;
  array INVEC, OUTVEC ;
    integer array TOTEVEC ;
    integer procedure SETFUNC ;
  integer n, k ;
begin comment MATHSORT is a fast sorting algorithm which
    produces a monotone rearrangement of an arbitrarily ordered
    set of n numbers (represented by the vector INVEC) by a
    surprising though familiar device. The resultant sorted set is
    represented by the vector OUTVEC. The key field, i.e. the
    ordered set of bits (or bytes) on which the sort is to be done,
    is obtained by some extraction-justification function denoted
    SETFUNC. The key field allows the representation of k pos-
    sible values denoted 0, 1, . . . , k-1.
      The procedure determines first of all the exact frequency
    distribution of the set with respect to the key, i.e. the number
    of elements of INVEC with key field value precisely equal to
    j for all j between 0 and k-1. The cumulative frequency dis-
    tribution TOTEVEC [i] ≡ ∑(j=0 to i) (Number of elements of
    INVEC with key value = j) is then computed for 0 ≦ i ≦ k-1.
    This induces the direct assignment (storage mapping func-
    tion) of each element of INVEC to a unique cell in OUTVEC.
    This assignment (like the determination of the frequency
    distribution) requires just one inspection of each element of
    INVEC. Thus the algorithm requires only 2n "look and do"
    operations plus k-1 additions (to get the cumulative fre-
    quency distribution).
      The algorithm can be easily and efficiently extended to
    handle alphabetic sorts or multiple key sorts. To sort on
    another key the same algorithm is applied to each new key
    field with the new INVEC designated as the last induced
    ordering (i.e. the current OUTVEC). The algorithm has been
    used extensively at LAS on binary as well as decimal machines
    both for internal memory sorts and (with trivial modification)
    for large tape sorts ;
  for i := 1 step 1 until n do
      TOTEVEC[SETFUNC(INVEC[i])] := TOTEVEC
        [SETFUNC(INVEC[i])] + 1 ;
  for i := 1 step 1 until k-1 do
      TOTEVEC[i] := TOTEVEC[i] + TOTEVEC[i-1] ;
  for i := 1 step 1 until n do
      begin OUTVEC[TOTEVEC[SETFUNC(INVEC[i])]]
          := INVEC[i] ;
        TOTEVEC[SETFUNC(INVEC[i])] :=
          TOTEVEC[SETFUNC(INVEC[i])] - 1 ;
        end
end MATHSORT.
```

CERTIFICATION OF ALGORITHM 23
MATHSORT (Wallace Feurzeig, *Comm. ACM*, Nov., 1960)
RUSSELL W. RANSHAW
University of Pittsburgh, Pittsburgh, Pa.

The MATHSORT procedure as published was coded for the IBM 7070 in FORTRAN. Two deficiencies were discovered:

1. The TOTVEC array was not zeroed within the procedure. This led to some difficulties in repeated use of the procedure.

2. Input vectors already in sort on nonsort fields were unsorted. That is, given the sequence

31, 21, 32, 22, 33,

Mathsort would produce, for a sort on the 10's digit:

22, 21, 33, 32, 31,

which is definitely out of sequence.

The following modified form of the procedure corrects these difficulties. Note the transformation of symbols.

```
procedure MATHSORT (I, O, T, n, k, S); value n, k;
          array I, O; integer array T; integer procedure S;
          integer n, k;
begin     for i := 0 step 1 until k - 1 do T[i] := 0;
          for i := 1 step 1 until n do T[S(I[i])] := T[S(I[i])] + 1;
          for i := k - 2 step -1 until 0 do T[i] := T[i] +
          T[i + 1];
          for i := 1 step 1 until n do
              begin O[n + 1 - T[S(I[i])]] := I[i];
                    T[S(I[i])] := T[S(I[i])] - 1;
              end
end MATHSORT.
```

Using the MATHSORT procedure ten times and having the procedure S supply each digit in order, 1000 random numbers of 10 digits each were sorted into sequence in 31 seconds. The method of locating the lowest element, interchanging with the first element, and continuing until the entire list has been so examined yielded a complete sort on the same 1000 random numbers in 227 seconds. Using the Table-Lookup-Lowest command in the 7070 yielded 56 seconds for the same set of random numbers.

ALGORITHM 24

SOLUTION OF TRI-DIAGONAL LINEAR EQUATIONS

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```
procedure TRIDAG (n, A, B, C, D) ; integer n ;
array A, B, C, D ;
comment: This procedure[1] finds the solution of an n × n system
    of linear equations whose matrix is in tridiagonal form, that
    is, a[i,j] = 0 for |i − j| ≧ 2. Parameters are: the main diagonal
    B[p], the diagonal just below A[r], the diagonal just above C[r],
    the right-hand side D: (where p = 1, ... , n and r = 1, ... ,
    n − 1) and the matrix order n. The solution vector replaces
    the input vector D and the vector B is also destroyed in the
    process ;
begin
    real w ; integer j ;
    D[1] := D[1]/B[1] ; w := B[1] ;
    for j := 2 step 1 until n do
        begin B[j − 1] := C[j − 1]/w ; w := B[j] − A[j − 1]
          × B[j − 1] ;
            D[j] := (D[j] − A[j − 1] × D[j − 1])/w end ;
    for j := 1 step 1 until n − 1 do
        D[n − j] := D[n − j] − B[n − j] × D[n − j + 1]
end TRIDAG
```

[1] D. W. PEACEMAN AND H. H. RACHFORD, JR., The Numerical Solution of Parabolic and Elliptic Differential Equations, Journal of the Soc. for Ind. and Applied Math. Vol. 3 March 1955.

ALGORITHM 25
REAL ZEROS OF AN ARBITRARY FUNCTION

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```
procedure ZEROS(n, C, FUNCTION, m, ep1, ep2, ep3, eta) ;
integer n, m ; real ep1, ep2, ep3, eta ; array C ;
procedure FUNCTION ;
comment: This procedure finds the real zeros of an arbitrary
    function using Muller's method[1, 2] and is adapted from a
    FORTRAN code by Frank.[3] Each iteration determines a zero
    of the quadratic passing through the last three function
    values. Parameters include the number of roots desired n.
    If Ci is zero, starting values are −1, 1, 0 respectively. If
    Ci = β then the starting values are .9β, 1.1β, β. The procedure
    FUNCTION(rt, frt) must be supplied to evaluate the func-
    tion value frt, given the argument rt. m is the maximum
    number of iterations permitted. ep1 is the relative conver-
    gence criterion on successive iterates. ep2 is the absolute
    convergence criterion on the function value. eta is the spread
    for multiple roots, that is, if |rt − Ci| < ep3 where Ci is a
    previously found root, then rt is replaced by rt + eta ;
begin integer L, jk, i, mm ; real p, p1, p2, x0, x1, x2, rt,
                frt, fprt, d, dd, di, h, bi, den, dn, dm, tem ;
    switch S : S1, S2, S3, S4 ;
    for L := 1 step 1 until m do
    begin jk := 0 ; if C[L] = 0 then go to initial else
    go to assign ;
initial: p := −1 ; p1 := 1 ; p2 := 0 ; go to start ;
assign: p := .9 × C[L] ; p1 := 1.1 × C[L] ; p2 := C[L] ;
start: rt := p ; go to fn ;
enter: go to S[if jk < 4 then jk else 4] ;
S1: rt := p1 ; x0 := fprt ; go to fn ;
S2: rt := p2 ; x1 := fprt ; go to fn ;
S3: x2 := fprt ; h := if C[L] = 0 then −1
    else −.1 × C[L] ; d := −.5 ;
loop: dd := 1 + d ; bi := x0 × d↑2 − x1 × dd↑2 × x2 ×
        (dd + d) ;
    den := bi↑2 − 4 × x2 × d × dd × (x0 × d − (x1 × dd) + x2) ;
    if den ≦ 0 then den := 0 else den := sqrt(den) ;
    dn := bi + den ; dm := bi−den ;
    if abs(dn) ≦ abs(dm) then den := dm else den := dn ;
    if den = 0 then den := 1 ;
    di := −2 × x2 × dd/den ; h := di × h ; rt := rt + h ;
    go to if abs(h/rt) < ep1 then call else fn ;
S4: if abs(fprt) < abs(x2 × 10) then
     begin x0 := x1 ; x1 := x2 ; x2 := fprt ; d := di ;
     go to loop end else begin di := di × .5 ; h := h × .5 ;
     rt := rt− h ; go to fn end ;
fn: jk := jk + 1 ; if jk < m then mm := 1 else mm := 0 ;
call: FUNCTION(rt, frt) ; if mm = 1 then go to compute
    else go to root ;
compute: fprt := frt ;
    for i := 2 step 1 until L do
    begin tem := rt− C[i− 1] ; if abs(tem) < ep3 then go to
    change else fprt := fprt/tem end
test: if abs(frt) < ep2 ∧ abs(fprt) < ep2 then go to root
    else go to enter ;
change: rt := rt + eta ; jk := jk− 1 ; go to fn ;
root: C[L] := rt end L
end ZEROS
```

[1] D. E. MULLER, A Method for Solving Algebraic Equations Using an Automatic Computer, *MTAC 10* (1956).

[2] W. L. FRANK, Finding Zeros of Arbitrary Functions, *J. ACM 5* (1958).

[3] W. L. FRANK, RWGRT, General Root Finder 704 FORTRAN Source Language Subroutine SHARE Distribution # 635. Parameters used by Frank are: ep1 = 10^{-6}, ep2 = 10^{-20}, ep3 = 10^{-20}, eta = 10^{-3}.

REMARK ON ALGORITHM 25
REAL ZEROS OF AN ARBITRARY FUNCTION
(B. Leavenworth, *Comm. ACM*, November 1960)

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On attempting to use this algorithm, I discovered the two following errors:

(1) The line following the SWITCH statement should read:
for L := 1 **step** 1 **until** n **do**

(2) The line starting with the label loop: should read:
loop: dd := 1 + d ; bi = x0 × d↑2 − x1 × dd↑2
+ x2 × (dd + d) ;

With these two modifications incorporated the algorithm was translated into the language of the Burroughs Algebraic Compiler and has been used successfully on the Burroughs 220 Computer.

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

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National Physical Laboratory, Teddington.

Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the *method* of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \cdots = a_5 = 0$, $a_6 = a_7 = \cdots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^6(x-1)^5(x-2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-44}. Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic.

This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, *is a very well-conditioned method of evaluation*. Knowing this, I was able to set a tolerance of 2^{-42} with confidence. If the *same function* had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $| x_{r+1} - x_r |$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$x = n\pi + y$$

$$\tan x - x = -n\pi + \frac{\frac{y^3}{3} - \frac{y^5}{30} - \cdots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^{60} - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable number of iterations are needed to find the root $x = 1$ Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is useful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4, that abs(fprt) < abs(x2 × 10), but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on the size of the function and on the size of the remainders r1 and r0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (Comm. ACM June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to *slow* convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root $x = -6.35099\,36103$ and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

[1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150–180.

ALGORITHM 26

ROOTFINDER III (Modification of Algorithm 15. Rootfinder II, Henry C. Thacher, Jr., *Comm. ACM*, August 1960)

JOHN G. HERRIOT, Stanford University, Stanford, California

```
procedure ROOTIII (f, a, eps, n, g, c, m) ; integer n, m ;
    real procedure f ; real a, eps, g, c ;
comment ROOTIII computes a value of g = y satisfying the
    equation y = f(y). The iteration will converge to Y providing
    that at some time in the iteration a g is reached such that
    abs(g − Y) × abs(d(df/dy)/dy) < 2 × abs((df/dy) − 1),
    where the derivatives are evaluated at Y. Input includes:
    (1) f, a procedure for computing f(y), (2) a, an initial ap-
    proximation to the root, (3) eps, a tolerance for the relative
    error in g, and (4) n, a maximum number of iterations to be
    performed. Output includes: (1) g, the required root, (2)
    c = f(g) − g, (3) m, a parameter indicating the success of
    the procedure. If the tolerance was not met m < 0. The num-
    ber |m| − 1 gives the number of times that the correction to g
    exceeded the preceding one. If f(y) − y has the same value
    for two successive approximations to g, then h = 1, and we
    exit to "alarm", a nonlocal label. Alarm should provide a
    means of deciding whether g is an acceptable root or not. ;
begin integer j ; real b, d, h ;
    m := 1 ; j := 0 ; c := 0 ;
    if f(0) = 0 then begin g := 0 ;
    go to return end ;
    g := f(a) ; b := d := c := g − a ;
    if c = 0 then go to return ;
    for j := 1 step 1 until n do
    begin c := f(g) − g ;
        if abs(c) ≦ abs(g) × eps then go to return ;
        h := b/c ;
        if h = 1 then go to alarm ;
    if h > 0 ∧ h < 2 then m := m + 1 ;
    d := d/(h − 1) ; b := c ; g := g + d
end iteration ;
m := − m ; return : end
```

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

J. H. WILKINSON

National Physical Laboratory, Teddington.

Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the *method* of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \cdots = a_5 = 0$, $a_6 = a_7 = \cdots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^5(x-1)^5(x-2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-44}. Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic. This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, *is a very well-conditioned method of evaluation*. Knowing this, I was able to set a tolerance of 2^{-42} with confidence. If the *same function* had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $| x_{r+1} - x_r |$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$x = n\pi + y$$

$$\tan x - x = -n\pi + \frac{\frac{y^3}{3} - \frac{y^5}{30} - \cdots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^{30} - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable number of iterations are needed to find the root $x = 1$. Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is useful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4 that abs(fprt) < abs(x2 × 10), but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on

the size of the function and on the size of the remainders r1 and r0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (Comm. ACM June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to *slow* convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root x = −6.35099 36103 and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

[1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150–180.

ALGORITHM 27
ASSIGNMENT
ROLAND SILVER
MIT Lincoln Laboratory,* Lexington, Massachusetts

```
procedure Assignment(d, n, x) ; value n ; integer n ;
          array d ; integer array x ;
comment: Assignment determines that permutation x of the
          integers [1:n] for which the sum (i := 1(1)n) of
          the elements d[i, x[i]] of the n × n matrix d is a
          minimum. n ≧ 2. For more complete information
          see: An Algorithm for the Assignment Problem,
          Roland Silver, Comm. ACM, Nov. 1960, p. 605 ;
  begin
  switch Switch := NEXT, L1, NEXT1, MARK ;
  array a[1:n, 1:n] ;
  integer array c[1:n], cb[1:n], lambda[1:n], mu[1:n],
          r[1:n], y[1:n] ;
  integer cbl, cl, cl0, i, j, k, l, rl, rs, sw ;
  comment:
INITIALIZE ;
  for i := 1 step 1 until n do
    begin min := d[i, 1] ;
    for j := 2 step 1 until n do if d[i, j] < min then min
      := d[i, j] ;
    for j := 1 step 1 until n do a[i, j] := d[i, j] − min
    end i ;
  for j := 1 step 1 until n do
    begin min := a[1, j] ;
    for i := 2 step 1 until n do if a[i, j] < min then min
      := a[i, j] ;
    for i := 1 step 1 until n do a[i, j] := a[i, j] − min
    end j ;
  for i := 1 step 1 until n do x[i] := y[i] := 0 ;
  for i := 1 step 1 until n do
    begin
    for j := 1 step 1 until n do
      begin
      if a[i, j] ≠ 0 ∨ x[i] ≠ 0 ∨ y[j] ≠ 0 then go to J1 ;
      x[i] := j ; y[j] := i
J1:   end j ;
    end i ;
START: comment: Start labeling ;
    rl := cl := 0 ; rs := 1 ;
    for i := 1 step 1 until n do
      begin mu[i] := lambda[i] := 0 ;
      if x[i] ≠ 0 then go to I1 ;
      rl := rl + 1 ; r[rl] := i ; mu[i] := −1
I1:   end i ;
LABEL: comment: Label and scan ;
    i := r[rs] ; rs := rs + 1 ;
    for j := 1 step 1 until n do
      begin if a[i, j] ≠ 0 or lambda[j] ≠ 0 then go
        to J2 ;
      lambda[j] := i ; cl := cl + 1 ; c[cl] := j ;
      if y[j] = 0 then go to MARK ;
      rl := rl + 1 ; r[rl] := y[j] ; mu[y[j]] := i
J2:   end j ;
      if rs ≦ rl then go to LABEL ;
      comment:
RENORMALIZE ;
  sw := 1 ; cl0 := cl ; cbl := 0 ;
  for j := 1 step 1 until n do
    begin if lambda[j] ≠ 0 then go to J3 ;
    cbl := cbl + 1 ; cb[cbl] := j
J3:   end j ;
  min := a[r[i], cb[i]] ;
  for k := 1 step 1 until rl do
    begin
    for l := 1 step 1 until cbl do if a[r[k], cb[l]] ≦ min
      then min := a[r[k], cb[l]]
    end k ;
  for i := 1 step 1 until n do
    begin if mu[i] ≠ 0 then go to I2 ;
    for l := 1 step 1 until cl0 do a[i, c[l]] := a[i, c[l]] + min ;
    go to I3 ;
I2:   for l := 1 step 1 until cbl do
      begin a[i, cb[l]] := a[i, cb[l]] − min ;
    go to Switch[sw] ;
NEXT: if a[i, cb[l] ≠ 0 ∨ lambda[cb[l]] ≠ 0 then go to L1 ;
    lambda[cb[l]] := i ;
    if y[cb[l]] = 0 then
      begin j := cb[l] ; sw := 2 ; go to L1 end ;
    cl := cl + 1 ; c[cl] := cb[l] ;
    rl := rl + 1 ; r[rl] := y[cb[l]] ;
L1:   end l ;
I3:     end i ;
    go to Switch[sw + 2] ;
NEXT1: if cl0 = cl then go to LABEL ;
    for i := cl0 + 1 step 1 until cl do mu[y[c[i]]] := c[i] ;
    go to LABEL ;
MARK: comment: mark new column and permute ;
    y[j] := i := lambda[j] ;
    if x[i] = 0 then begin x[i] := j ; go to
      START end ;
    k := j ; j := x[i] ; x[i] := k ;
    go to MARK
    end Assignment
```

* Operated with support from the U. S. Army, Navy and Air Force.

[NOTE: The reader should distinguish between the letter and the figure 1, both of which appear in the above algorithm.—Ed.]

CERTIFICATION OF ALGORITHM 27
ASSIGNMENT [Roland Silver, *Comm. ACM*, Nov. 1960]
ALBERT NEWHOUSE
University of Houston, Houston, Texas

The ASSIGNMENT algorithm was translated into MAD and successfully run on the IBM 709/7094 after the following corrections were made:

All references to array a and d refer to the same array, i.e. change all $a[i, j]$ to $d[i, j]$. Furthermore:

(a) 3rd line after *LABEL*: **comment**: Label and scan;
should read
begin if $d[i, j] \neq 0 \vee$ lambda $[j] \neq 0$ **then go**

(b) first line after *J3*: **end** *j*;
should read
$min := d[r[1], cb[1]]$;

(c) line *I2*:
should read
I2: **for** $l := 1$ **step** 1 **until** *cbl* **do**

Since there is no provision made for this algorithm to end the following additions were made:

(1) in the integer declaration add the variable: *flag*

(2) first line after *START*: **comment**: ···
add the line
$flag := n$;

(3) first line before *I1*: **end** *i*;
change to read
$rl := rl + 1$; $r[rl] := i$; $mu[i] := -1$; $flag := flag - 1$

(4) add a line after *I1*: **end** *i*;
if $flag = n$ **then go to** *FINI*;

(5) change the last line of the algorithm to read:
FINI: **end** Assignment

In order to obtain the minimum value of the $\sum_{i=1}^{n} a_{ix_i}$ (in the following called total) the following additions may be made:
Add a real variable *total* and

(A) new line after *INITIALIZE*;
$total := 0$;

(B) new line after the first **end** *i*;
$total := total + min$;

(C) new line after the first **end** *j*;
$total := total + min$;

(D) after the line **end** *k*; after *J3*: **end** *i*;
add the line
$total := total + (rl+cbl-n) \times min$;

CERTIFICATION OF ALGORITHM 27 ASSIGNMENT [Roland Silvers, *Comm. ACM 3*, Nov. 1960].

ROBERT D. WITTY
Burroughs Corp., Detroit, Mich.

Assignment was successfully run on the Burroughs B5000 using Burroughs extended ALGOL 60.

Input Array

60	0	0	76	0	0
0	40	18	0	60	24
60	16	2	4	0	40
0	27	18	3	55	75
0	40	62	16	11	53
28	4	10	84	0	16

Solution Vector: $X(6, 4, 3, 1, 5, 2)$

The following changes were made in the algorithm prior to its successful run:

FROM $MIN := a[r[i], cb[i]]$;
TO $MIN := a[r[1], cb[1]]$;

FROM **if** $X[i] = 0$ **then begin** $X[i] := j$;
go to *START* **end**;
TO **if** $X[i] = 0$ **then begin** $X[i] := j$;
for $i := 1$ **step** 1 **until** N **do begin if** $X[i] = 0$ **then go to** *START*;
end; **go to** *EXIT*; **end**;

FROM **end** *ASSIGNMENT*
TO *EXIT*: **end**; *ASSIGNMENT*

ALGORITHM 28
LEAST SQUARES FIT BY ORTHOGONAL POLYNOMIALS

JOHN G. MACKINNEY
General Kinetics Incorporated, Arlington 6, Virginia

```
procedure  LSFIT (f, x1, xm, m, k, alpha, beta, sigma, s, p)  ;
           value x1, xm, m, k  ; real x1, xm  ; integer
             m, k  ;
           real array f, alpha, beta, sigma, s, p  ;
comment  LSFIT accepts m values of the function f at equal
    intervals of the abscissa from x1 through xm, and obtains in
    p[0] through p[k] the coefficients of the best polynomial ap-
    proximation of degree k or less (least squares) as programmed
    by George E. Forsythe, Journal SIAM 5, no. 2, June 1957,
    with only minor variations. The output values alpha [1:k],
    beta [0:k], and s [0:k] enable the user to make final adjust-
    ments to the results, according to the statistic sigma [0:k].
    LSFIT uses the procedure POLYX (a, b, c, d, n) to trans-
    form its results from the interval (−2, 2) to the interval (x1,
    xm)  ;
begin integer  i, j  ; real dummy, x, xone, deltax, delsq,
                 omega, lastw, thisw  ;
               real array cthisp, cpoly [0:k], clastp [−1:k],
                 lastp, thisp [1:m]  ;
               Boolean swx  ;
comment  Initialization  ;
    swx := true  ; beta [0] := clastp [0] := clastp [−1] :=
      delsq := omega := 0  ;
    cthisp [0] := 1  ; thisw := m  ;
    for i := 1 step 1 until m do
    begin delsq := delsq + f[i]↑2  ;
        thisp [i] := 1  ; lastp [i] := 0  ;
        omega := omega + f[i] end  ;
    s [0] := cpoly [0] := omega/thisw  ;
    delsq := delsq − s [0] × omega  ;
    sigma [0] := delsq/(m−1)  ;
comment  Transformation of abscissa  ; i := m + 2  ;
           if 2×i = m then deltax := 4/(m − 1) else deltax :=
             4/m  ; xone := −2  ;
comment  Main Computation loop  ;
           for i := 0 step 1 until k−1 do
           begin dummy := 0  ; x := xone  ;
           1:  for j := 1 step 1 until m do
           begin dummy := dummy + x × thisp [j] ↑ 2  ;
           x := x + deltax end  ;
           2:  alpha [i + 1] := dummy/thisw  ;
               lastw := thisw  ;
               thisw := omega := 0  ;
               x := xone  ;
           3:  for j := 1 step 1 until m do
           begin dummy := beta [i] × lastp [j]  ;
               lastp [j] := thisp [j]  ;
               thisp [j] := (x − alpha [i + 1]) × thisp [j]
                 −dummy  ;
               thisw := thisw + thisp [j] ↑ 2  ;
               omega := omega + f [j] × thisp [j]  ;
               x := x + deltax end  ;
           4:  beta [i + 1] := thisw / lastw  ;
               s[i + 1] := omega / thisw  ;
                 delsq := delsq − s[i + 1] × omega  ;
               sigma [i + 1] := delsq / (m − i − 1)  ;
               if swx then go to 6  ;
           5:  cpoly [i + 1] := 0  ; go to 9  ;
comment  Termination of main loop when higher power will
           not improve fit  ;
           6:  if sigma [i + 1] < sigma [i] then go to 7  ;
               swx := false  ; go to 5  ;
comment  Recursion for polynomial coefficients  ;
           7:  for j := 0 step 1 until i do
               begin dummy := clastp [j] × beta [i]  ;
               clastp [j] := cthisp [j]  ;
cthisp [j] := clastp [j − 1] − alpha [i + 1] × cthisp [j] − dummy  ;
cpoly [j] := cpoly [j] + s [i + 1] × cthisp [j] end  ;
    8:  cpoly [i + 1] := s [i + 1]
    cthisp [i + 1] := 1  ;
    9:  clastp [i + 1] := 0 end of main
computation loop, transformation of polynomial follows  ;
    begin real a, b  ;
    a := deltax × (m − 1) / (xm − x1)  ;
    b := xone − a × x1  ;
    POLYX (a, b, cpoly, p, k) end
end of LSFIT
```

REMARK ON ALGORITHM 28
LEAST-SQUARES FIT BY ORTHOGONAL POLYNOMIALS (John G. MacKinney, *Comm. ACM 3* (Nov. 1960))

D. B. MACMILLAN
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The algorithm obtains the coefficients of the fitted polynomial of lowest degree such that an increase in the degree would cause an increase in the statistic sigma (sigma squared in Forsythe's notation). A significant decrease in sigma, as one goes from a fitted polynomial to one of higher degree, indicates that the increase in degree causes an improvement in the fit to the function underlying the data, rather than merely following more closely the random variations about that function introduced by the physical measurement process.

If one of the orthogonal polynomials, say the one of ith degree, is missing from the underlying function, and some of the orthogonal polynomials of higher degree are present, then the fitted polynomial of ith degree will not be a real improvement over that of $(i - 1)$-th degree, but higher order fitted polynomials will be a real improvement. For example, in one of our recent routine problems the coefficient of the second degree orthogonal polynomial was quite small, and the first few values of sigma, starting with sigma (1), were .255, .264, .062, .046, .048. The algorithm would have chosen the first degree fitted polynomial as "best", but the third and fourth degree fitted polynomials were clearly better than it.

This loophole may be plugged by modifying the algorithm so it computes the coefficients of the polynomial of lowest degree i for which it is true that

$$\text{sigma } (i + 1) \geq \text{sigma } (i)$$

and that

$$\text{sigma } (j) \geq .6 \text{ sigma } (i) \qquad j = i+2, i+3, \cdots, k,$$

(.6 was chosen arbitrarily).

REMARK ON ALGORITHM 28 [E2] LEAST SQUARES FIT BY ORTHOGONAL POLYNOMIALS [John G. MacKinney, *Comm. ACM 3* (Nov. 1960), 604]

G. J. MAKINSON (Recd. 30 Sept. 1965, 29 Aug. 1966 and 7 Nov. 1966)
University of Liverpool, Liverpool 3, England

There are three errors in the published procedure.

Line 32 $i := m + 2$; should read $i := m \div 2$;

Line 56 *delsq*/($m-i-1$); should read *delsq*/($m-i-2$);

Line 69 ; is missing from end of statement *cpoly*[$i+1$] := *s*[$i+1$];

Three improvements can be made to the procedure. In the case of equally spaced points, it is possible to center them about the origin; all alphas are then zero. This is achieved by replacing the statements on lines 32, 33, and 34 by *deltax* := 4/($m-1$); *xone* := -2; All statements involving alphas can then be revised.

Another improvement can be made by deleting the two statements on line 37 and all of lines 38, 39, and 40. These statements are completely redundant.

The third improvement is to rewrite line 71 to read

clastp[$i+1$] := 0; 9: **end** *of main*

instead of

9: *clastp*[$i+1$] := 0 **end** *of main*

ALGORITHM 29
POLYNOMIAL TRANSFORMER
JOHN G. MACKINNEY
General Kinetics Inc., Arlington 6, Virginia

```
procedure  POLYX (a, b, c, d, n)  ;  value a, b, n  ;  integer
             n  ;  real  a,  b  ;
           real array c, d  ;
comment  POLYX computes coefficients d0, d1, ... , dn of the
           transformed polynomial p(t) given c0, c1, ... ,
           cn of p(x) where x = at + b  ;
begin integer i, j, k  ;  real array z, w [0:n]  ;
    w[0] := z[0] := 1  ;  d[0] := c[0]  ;
    for i := 1 step 1 until n do
        begin w[i] := 1  ;  z[i] := b × z[i − 1]  ;
          d[0] := d[0] + c[i] × z[i]
        end of initialization  ;
    for j := 1 step 1 until n do
        begin w[0] := w[0] × a  ;  d[j] := c[j] × w[0]  ;
          k := 1  ;
            for i := j + 1 step 1 until n do
                begin w[k] := a × w[k] + w[k − 1]  ;
                    d[j] := d[j] + c[i] × w[k] × z[k]  ;
                    k := k + 1 end
end
end  of POLYX polynomial transformer
```

ALGORITHM 30

NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION

K. W. ELLENBERGER

Missile Division, North American Aviation, Downey, California

```
procedure ROOTPOL (n, a, L, F, u, v, CONV) ;
          value n, a, L, F ; integer L, F, n ;
          array a, u, v, CONV ;
```

comment The Bairstow and Newton correction formulae are used for a simultaneous linear and quadratic iterated synthetic division. The coefficients of a polynomial of degree n are given as a_i ($i = 0, i, \ldots, n$) where a_n is the constant term. The coefficients are scaled by dividing them by their geometric mean. The Bairstow or Newton iteration method will nearly always converge to the number of figures carried, F, either to root values or to their reciprocals. If the simultaneous Newton and Bairstow iteration fails to converge on root values or their reciprocals in L iterations, the convergence requirement will be successively reduced by one decimal figure. This program anticipates and protects against loss of significance in the quadratic synthetic division. (Refer to "On Programming the Numerical Solution of Polynomial Equations," by K. W. Ellenberger, Commun. ACM *3* (Dec. 1960), 644-647.) The real and imaginary part of each root is stated as u[i] and v[i], respectively, together with the corresponding constant, $CONV_i$, used in the convergence test. This program has been used successfully for over a year on the Bendix G15-D (Intercard System) and has recently been coded for the IBM 709 (Fortran System);

```
          begin integer i, j, m ; array h, b, c, d, e[-2 :n] ;
              real t, K, ps, qs, pt, qt, s, rev, r ;
ROOTPOL:  b_-1 := b_-2 := c_-1 := c_-2 := d_-1 := d_-2 := e_-1 :=
            e_-2 := 0 ;
          for j := 0 step 1 until n do h_j := a_j ; t := 1 ;
            K := 10^F ;
ZROTEST:  if h_n = 0 then
          begin u_n := 0 ; v_n := 0 ; CONV_n := K ;
            n := n - 1 ; go to ZROTEST
          end ;
INIT:     if n = 0 then go to RETURN ;
            ps := qs := pt := qt := s := 0 ;
            rev := 1 ; K := 10^F ;
          if n = 1 then
          begin r := - h_1/h_0 ; go to LINEAR
          end ;
          for j := 0 step 1 until n do
          begin
          if h_j = 0 then s := s else s := s + log(abs(hj))
          end ; s := s^10 ;
          for j := 0 step 1 until n do h_j := h_j/s ;
          if abs (h_1/h_0) < abs (h_n-1/h_n) then
REVERSE:  begin t := -t ; m := entier ((n+1)/2) ;
          for j := 0 step 1 until m do
          begin s := h_j ; h_j := h_n-j ; j_n-j := s
          end
          end ;
          if qs ≠ 0 then
          begin p := ps ; q := qs ; go to ITERATE
          end ;
          if h_n-2 = 0 then
          begin q := 1 ; p := -2
          end else
          begin q := h/h_n-2 ; p := (h_n-1 - q × h_n-3)/h_n-2
          end ;
          if n = 2 then go to QADRTIC ; r := 0 ;
ITERATE:  for i := 1 step 1 until L do
          begin
BAIRSTOW: for j := 0 step 1 until n do
          begin b_j := h_j - p × b_j-1 - q × b_j-2 ;
            c_j := b_j-p × c_j-1 - q × c_j-2
          end ;
          if n_n-1 = 0 then go to BNTEST ;
          if b_n-1 = 0 then go to BNTEST ;
          if abs (h_n-1/b_n-1)<K then go NEWTON ;
            b_n := h_n-q × b_n-2 ;
BNTEST:   if b_n = 0 then go to QADRTIC ;
          if K < abs (h_n/b_n) then go to QADRTIC ;
NEWTON:   for j := 0 step 1 until n do
          begin d_j := h_j + r × d_j-1 ; e_j := d_j + r × e_j-1
          end ;
          if d_n = 0 then go to LINEAR ;
          if K < abs (h_n/d_n) then go to LINEAR ;
            c_n-1 := -p × c_n-2 - q × c_n-3 ;
            s := c^2_n-2 - c_n-1 × c_n-3 ;
            if s=0 then
          begin p := p - 2 ; q := q × (q + 1)
          end else
          begin p := p + (b_n-1 × c_n-2 - b_n × c_n-3)/s ;
            q := q + (-b_n-1 × c_n-1 + b_n × c_n-2)/s
          end ;
          if e_n-1 = 0 then r := r-1 else r := r - d_n/e_n-1
          end ; ps := pt ; qs := qt ; pt := p ;
            qt := q ;
          if rev < 0 then K := K/10 ; rev = -rev ;
            go to REVERSE ;
LINEAR:   if t < 0 then r := 1/r ; u_n := r ; v_n := 0 ;
          CONV_n := K ; n := n-1 ;
          for j := 0 step 1 until n do h_j := d_j ;
          if n = 0 then go to RETURN ;
            go to BAIRSTOW ;
QADRTIC:  if t < 0 then
          begin p := p/q ; q := 1/q
          end ;
          if 0 < (q - (p/2)^2) then
          begin u_n := u_n-1 := -p/2 ;
            s := sqrt (q - (p/2)^3) ; v_n := s ;
            v_n-1 := -s
          end else
          begin s := sqt ((p/2)^2) - q) ;
          if p < 0 then u_n := -p/2 + s
            else u_n := -p/2-s ; u_n-1 := q/u_n ;
            v_n := v_n-1 := 0
          end ; CONV_n := CONV_n-1 := K ;
            n := n-2 ;
            for j := 0 step 2 until n do h_j := b_j ;
            go to INIT ;
RETURN:   end
```

CERTIFICATION OF ALGORITHM 30 NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION (K. W. Ellenberger, *Comm. ACM*, Dec. 1960)

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ROOTPOL was coded by hand for the LGP-30 using the ACT-III Compiler with 24 bits of significance. The following corrections were found necessary.

(a) $b_{-1} := b_{-2} := c_{-1} := c_{-2} := d_{-1} := d_{-2} := e_{-1} := e_{-2} := 0$ *should be*
$b_{-1} := b_{-2} := c_{-1} := c_{-2} := d_{-1} := e_{-1} := h_{-1} := 0$

(b) m := entier ((n + 1)/2) *should be*
m := entier ((n − 1)/2)

(c) $j_{n-j} := s$ *should be* $h_{n-j} := s$

(d) $q := h/h_{n-2}$ *should be* h_n/h_{n-2}

(e) $cj := b_j - p \times c_j - 1 - q \times c_{j-2}$ *should be*
$c_j := b_j - p \times c_{j-1} - q \times c_{j-2}$

(f) **if** $n_{n-1} = 0$ **then go to** BNTEST *should be*
if $h_{n-1} = 0$ **then go to** BNTEST

(g) s := sqrt (q − (p/2)³) *should be*
s := sqrt (q − (p/2)²)

(h) **for** j := 0 **step** 2 **until** n **do** $h_j := b_j$ *should be*
for j := 0 **step** 1 **until** n **do** $h_j := b_j$

(i) **go to** BAIRSTOW *should be* **go to** ITERATE

The following correction was found necessary in the given example (Refer to "On Programming the Numerical Solution of Polynomial Equations," by K. W. Ellenberger, *Comm. ACM 3*, Dec., 1960):

$f(x) = (.10098).10^8\ x^4 - (.98913)\ 10^6\ x^2 + (.10000)\ 10^6\ x + (.10000)\ 10^1 = 0$ *should be*
$f(x) = (.10098)\ 10^8\ x^4 - (.98913)\ 10^6\ x^3 - (.10990)\ 10^6\ x^2 + (.10000)\ 10^6\ x + (.10000)\ 10^1 = 0$

With these corrections the results obtained agree with those given in the example.

For equations of higher order it was found necessary to avoid repeated scaling of the reduced equation in order to prevent floating point overflow. The range on the exponent in the ACT III system is $-32 \leqq e \leqq 31$.

Further floating point overflow difficulties were experienced when certain coefficients in the reduced equation became small but not zero. The following additions were made to avoid this fault:

(a) **for** j := 0 **step** 1 **until** n **do** $h_j := d_j$ *was replaced by*
for j := 0 **step** 1 **until** n **do begin if** abs $(h_j/d_j) < K$ **then** $h_j := d_j$ **else** $h_j := 0$ **end**

(b) **for** j := 0 **step** 1 **until** n **do** $h_j := b_j$ *was replaced by*
for j := 0 **step** 1 **until** n **do** begin **if** abs $(h_j/b_j) < K$ **then** $h_j := b_j$ **else** $h_j := 0$ **end**

With the above changes the following results were obtained:

$x^4 - 3x^3 + 20x^2 + 44x + 54 = 0$
$x = -.9706390 \pm 1.005808i$
$x = 2.470639 \pm 4.640533i$

$x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$
$x = -.9999999 \pm .9999999i$
$x = 1.500000 \pm 1.322876i$
$x = .5000002 \pm .8660251i$

$x^5 + x^4 - 8x^3 - 16x^2 + 7x + 15 = 0$
$x = 3.000001$
$x = -2.000000 \pm 1.000001i$
$x = -.9999997$
$x = .9999998$

* Work supported by the U. S. Atomic Energy Commission

CERTIFICATION OF ALGORITHM 30 NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION [K. W. Ellenberger, *Comm. ACM 3* (Dec. 1960), as corrected in the previous Certification by William J. Alexander, *Comm. ACM 4* (May 1961)]

KALMAN J. COHEN
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The ROOTPOL procedure originally published by Ellenberger as corrected and modified by Alexander was coded for the Bendix G20 in 20-GATE. Some serious errors were found in the third and fourth lines above the statement labelled "REVERSE" in Ellenberger's Algorithm which were not mentioned in Alexander's Certification. First, the function "log" is not a standard function in ALGOL 60; it is clear from the context, however, that Ellenberger intends this to be the logarithm function to the base 10. Second, Ellenberger's Algorithm failed to divide the accumulated sum of the logarithms by n+1 before taking the antilogarithm.

The correct, and slightly simplified, manner in which the third and fourth lines above the statement labelled "REVERSE" should read is:

if $h_j \neq 0$ **then** s := ln(abs(h_j))
end; s := s/(n+1); s := exp(s);

With these corrections, the numerical results obtained essentially agree with those reported by Alexander.

CERTIFICATION OF ALGORITHM 30 [C2] NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION [K. W. ELLENBERGER, *Comm. ACM 3* (Dec. 1960), 643]

JOHN J. KOHFELD (Recd. 31 Aug. 1964, 18 Nov. 1964 and 10 Nov. 1966)
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The *ROOTPOL* procedure was found to use the identifiers *p*, *q*, without declaring them. They should be declared **real**.

The first ALGOL statement in Cohen's Certification [*Comm. ACM 5* (Jan. 1962), 50] which reads:

if $h_j \neq 0$ **then** $s := ln\ (abs(h_j))$

should read:

if $h_j \neq 0$ **then** $s := ln\ (abs(h_j)) + s$.

The next line could be simplified to read:

end; $s := exp(s/(n+1))$;

The above corrections, as well as Algorithm 30 itself, are in publication language ALGOL. In order to translate the algorithm to reference language ALGOL, which is now used in CACM, 10^F would need to be replaced by $10 \uparrow F$, and h_j would need to be replaced by $h\ [j]$.

With these corrections and those contained in Alexander's Certification [*Comm. ACM 4* (May 1961), 238], Ellenberger's Algorithm was adapted to B-5000 ALGOL and successfully executed on the Burroughs B-5000 computer at United Technology Center. The results from the four examples used by Alexander are given below.

Example 1

$(1.0098)10^7x^4 - (9.8913)10^5x^3 - (1.0990)10^5x^2 + 10^5x + 1 = 0.$

The roots are:

$x = -0.201080185406$

$x = 0.149521622653 \pm 0.163989609283i$

$x = (-9.99989011230)10^{-6}.$

Example 2

$x^4 - 3x^3 + 20x^2 + 44x + 54 = 0$

$x = 2.47063897001 \pm 4.64053316164i$

$x = -0.970638970010 \pm 1.00580758903i$

Example 3

$x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$

$x = -0.999999999990 \pm 1.000000000000i$

$x = 1.500000000000 \pm 1.32287565553i$

$x = 0.500000000000 \pm 0.866025403780i$

Example 4

$x^5 + x^4 - 8x^3 - 16x^2 + 7x + 15 = 0$

$x = 3.00000000000$

$x = -2.00000000000 \pm 1.00000000003i$

$x = -0.999999999990$

$x = 1.000000000000$

These results agree substantially with those given in Alexander's Certification.

ALGORITHM 31
GAMMA FUNCTION

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Burroughs Corporation, Pasadena, California

```
real procedure Gamma (x); real x;
comment For x in the range 2 ≤ x ≤ 3 an approximating polynomial is used. In this range the maximum absolute error ε(x) is | ε(x) | < 0.25 × 10⁻⁷. For x > 3 we write Γ(x) = (x−1)(x−2) ...(x−n)Γ(x−n) where 2 ≤ (x−n) ≤ 3, and for x < 2 we write Γ(x) = Γ(x+n) / x(x+1)...(x+n−1) where 2 ≤ (x−n) ≤ 3. For x = 0 or a negative integer Γ(x) is set equal to a large value 10⁵⁰.
begin
  real h, y;
  h := 1.0;  y := x;
A1: if y = 0 then h := 10⁵⁰
    else if y = 2.0 then go to A2
    else if y < 2.0 then begin
    h := h/y;  y := y + 1.0;  go to A1 end
    else if y ≥ 3.0 then begin
    y := y − 1.0;  h := h × y;  go to A1 end
    else begin y := y − 2.0;
    h := (((((((.0016063118 × y + .0051589951) × y
      + .0044511400) × y + .0721101567) × y
      + .0821117404) × y + .4117741955) × y
      + .4227874605) × y + .9999999758) × h end;
A2: Gamma := h end Gamma.
```

CERTIFICATION OF ALGORITHM 31
GAMMA FUNCTION [R. M. COLLINGE, *Comm. ACM*, Feb. 61]

PETER G. BEHRENZ
Mathematikmaskinnämnden, Stockholm, Sweden

GAMMA was successfully run on FACIT EDB using FACIT-ALGOL 1, which is a realization of ALGOL 60 for FACIT EDB. No changes in the program were necessary. The relative error was as stated in the comment of GAMMA about 10^{-8}.

CERTIFICATION OF ALGORITHM 31
GAMMA FUNCTION [R. M. Collinge, *Comm. ACM*, Feb. 61]

PETER G. BEHRENZ
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ALGORITHM 32
MULTINT

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```
real procedure MULTINT (n, Low, Upp, Funev, s, P, u, w);
        value n;
        real procedure Low, Upp, Funev; array s, u,
        w; integer n;
comment MULTINT will perform a single, double, triple,...,
  T-order integration depending on whether n=1, 2,..., T. The
  result is:
```

$$\text{MULTINT} = \int_{\text{Low}(1)}^{\text{Upp}(1)} \text{Funev}(1, x_1)\,dx_1 \int_{\text{Low}(2,x_1)}^{\text{Upp}(2,x_1)} \text{Funev}(2,x_1,x_2)\,dx_2 \ldots \int_{\text{Low}(n,x_1,\ldots,x_{n-1})}^{\text{Upp}(n,x_1,\ldots,x_{n-1})} \text{Funev}(x_1,\ldots,x_n)\,dx_n$$

```
  The variable of integration is x[j]. j=1 refers to the outermost
  integral, j=n, the innermost integral. The code divides each
  interval equally into s[j] subintervals and performs a P-point
  Gaussian integration on each subinterval with weight functions
  w[k[j]] and abscissas u[k[j]]. P is the size of the arrays of
  weight functions and abscissas and must be provided by the
  main code along with these arrays.
    Since the values x[1], x[2],..., x[n], are stored in an array, as
  are a, b, c, d, r, it is necessary to substitute an integer for the
  upper bound T of these arrays before the program is executed.
  This means, for example, if 3 is substituted for T, then the
  procedure will not do a 4th order integral unless it is retrans-
  lated with T ≥ 4.
    The values of the lower and upper bounds and functions must
  of course be specified at the time of use. If each of these con-
  stituted a separate procedure, it would require writing and
  translating 3n different procedures. This is eliminated by group-
  ing them into Low, Upp, and Funev which compute the lower
  and upper bounds and value of the functions respectively in
  each of the jth integrals. Since these are each essentially a col-
  lection of "subprocedures," the first statement of each should
  be a switch directing the code to the "subprocedure" which is
  used in the jth integral. Note that, for example, Low(3,x) is
  formally a function of x[1], x[2],..., x[T]; this is done merely
  because it is more convenient to make Low(j,x) formally a func-
  tion of the whole array x for all j. Actually of course Low(3, x)
  would be a function of x[1] and x[2] only;
begin   real array a, b, c, d, r, x[1:T];
        integer array k, h[1:T]; real f; integer j, m;
        for j :=1 step 1 until T do
            x[j] := 0.0;
        m := 1;
        r[n+1] := d[n+1] := 1.0;
setup:  for j := m step 1 until n do
        begin
          a[j] := Low(j,x);
          b[j] := Upp(j,x);
          d[j] := (b[j]- a[j])/s[j];
          c[j] := a[j] + 0.5 × d[j];
          x[j] := c[j] + 0.5 × d[j] × u[1];
          r[j] := 0.0;
          h[j] := k[j] := 1; end;
          j := n;
sum:    f := Funev(j,x);
        r[j] := r[j] + r[j+1] × d[j+1] × f × w[k[j]];
        if (k[j] < P) then go to labk;
        if (h[j] < s[j]) then go to labh;
        j := j-1;
        if (j = 0) then go to exit;
        go to sum;
labh:   h[j] := h[j] + 1;
        c[j] := a[j] + (h[j] - 0.5) × d[j];
        k[j] := 1;
        go to initalx;
labk:   k[j] := k[j] + 1;
initalx: x[j] := c[j] + 0.5 × d[j] × u[k[j]];
        if (j=n) then go to sum;
        m := j+1;
        go to setup;
exit:  MULTINT := r[1] × d[1] × 0.5↑ n; end
```

CERTIFICATION OF ALGORITHM 32
MULTINT [R. Don Freeman, *Comm. ACM*, Feb. 1961]

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* Work supported by the U. S. Atomic Energy Commission.

The procedure was transcribed into the ACT-III language for the LGP-30 computer, and was tested on the integrals:

$$(1)\quad \int_0^1\int_0^1\int_0^1\int_0^1 k[\cos u - 7u \sin u - 6u^2 \cos u + u^3 \sin u]\,dw\,dx\,dy\,dz = \sin k$$

where $u = kwxyz$, and

$$(2)\quad \int_0^1\int_0^{\sqrt{1-x^2}}\int_0^{\sqrt{1-x^2-y^2}} \frac{dz\,dy\,dx}{x^2+y^2+(z-k)^2} = \pi\left(2 + \frac{1}{2}\left(\frac{1}{k} - k\right)\log\left|\frac{1+k}{1-k}\right|\right).$$

The ALGOL procedures for the second integral are:

```
real procedure Low (j,x);
Low := 0;
real procedure Upp(j,x); comment z ≡ x[3], y ≡ x[2], x ≡
  x(1);
begin
integer i; real temp;
temp := 1.0;
for i := j-1 step - 1 until 1 do
temp := temp - x[j] × x[j];
Upp := sqrt(temp)
end;
real procedure Funev(j,x);
comment The real parameter k is global;
Funev := if j < 3 then 1.0 else 1/(x[1]×x[1]+x[2]×x[2]+(x[3]-k)
  ↑2);
```

The first integral was tested only with $s[j] = 1$, and with various Gaussian formulas for integrals over the interval $(-1,+1)$. Results were as follows:

k	$\pi/2$	π	$3\pi/2$	2π
true	1.0000000	0.0000000	−1.0000000	0.0000000
p = 2	0.993704	−0.0333603	+0.020166	6.881490
p = 3	1.000032	0.0000848	−1.061651	−0.597419
p = 4	0.999999	0.0000001	−0.998407	+0.0027035
p = 5	1.000000	−0.0000002	−1.000028	−0.0007857

For the second integral, two values of $s = s[1] = s[2] = s[3]$ were used, and two values of p. Results were as follows:

k	1/2		2	
true	11.46027376		1.10609687	
s	1	2	1	2
p = 2	5.454460	11.838651	1.0368770	1.1184305
p = 3	9.361666	12.408984	1.1343551	1.1094278

The effect of the pole at $(0,0,k)$ is obvious.

For the algorithm to run in any compiler, the semicolon following $x[T]$; in the fourth line above the end of the comment must be deleted. The array bounds on the arrays r and d must be increased to $[1 : T+1]$.

For a system which permits variable array bounds, the introduction of the integer T appears superfluous. For such a system, T may be replaced by n throughout with a probable gain in efficiency. For most translators, the presence of undefined elements in an array will not cause difficulties, provided these elements do not appear in an expression before they are assigned a value. The statement "**for** j := 1 **step** 1 **until** T **do** $x[j]$:= 0.0;" is thus superfluous. The semicolon before the **end** which precedes the label "*sum*" also appears unnecessary.

In spite of these minor corrections, the algorithm appears to be extremely convenient for multiple quadratures over arbitrary regions using the Cartesian product of any explicit one-dimensional formula (and not merely a Gaussian formula) for integrating over the range [−1,1]. If endpoints are used in the formula, it will, of course, repeat the calculation for each section of the range.

REMARKS ON ALGORITHM 32 [D1]
MULTINT [R. Don Freeman, Jr., *Comm. ACM 4* (Feb. 1961), 106]
AND
CERTIFICATION OF ALGORITHM 32 [Henry C. Thacher, Jr., *Comm. ACM 6* (Feb. 1963), 69]

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KEY WORDS AND PHRASES: numerical integration, multidimensional integration, Gaussian integration
CR CATEGORIES: 5.16

The real procedure *MULTINT* was corrected according to the certification. It was then compiled on a CDC 3800 computer and tested on the second integral given in the certification. It became apparent that

(i) Equation (2) of the certification should read

$$\int_{-1}^{1}\int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}}\int_{-\sqrt{1-x^2-y^2}}^{\sqrt{1-x^2-y^2}} \frac{dz\,dy\,dx}{x^2+y^2+(z-k)^2} = \pi\left(2+\left(\frac{1}{k}-k\right)\log\left|\frac{1+k}{1-k}\right|\right) \tag{2}$$

It should be noted that the right-hand side of equation (2) as printed in the certification does not correspond either to the original limits or to those given above.

(ii) the statement

$$Low := 0;$$

in the real procedure *Low* should be replaced by

$$Low := -Upp(j, x);$$

(iii) the second line of the **for** statement in the real procedure *Upp* should read

$$temp := temp - x[i] \times x[i];$$

After making these corrections, it is possible to obtain results corresponding to a permuted version of the table given in the certification, which should be replaced by the following:

k	½		2	
true	11.46027375		1.10609686	
s	1	2	1	2
$P = 2$	5.454466	9.361670	1.0368787	1.1184317
$P = 3$	11.838664	12.408983	1.1343568	1.1094294

In addition, since several compilers require specifications, it would be desirable

(i) to change the last specification in the heading of *MULTINT* to read

integer n, P;

(ii) to insert the specifications

integer j; **array** x;

in the heading of the real procedures *Low*, *Upp*, and *Funev*.

Some of these additions were necessary in order to ensure correct results with the compiler used for the tests.

ALGORITHM 33
FACTORIAL
M. F. LIPP
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```
real procedure Factorial (n) ;
        value n ; integer n ;
comment This procedure makes use of the implicitly defined
  recursive property of Algol to compute n!;
begin Factorial := if n = 0 then 1. else n× Factorial (n−1)
        end
```

ALGORITHM 34
GAMMA FUNCTION
M. F. LIPP
RCA Digital Computation and Simulation Group, Moorestown, New Jersey

```
real procedure Gamma (x) ; real x ;
comment This procedure generalizes the recursive factorial
  routine, finding Γ(1+x) for reasonable values of x. Accuracy
  vanishes for large x(|x| > 10) and for negative x with small
  fractional parts. For x being a negative integer the impossible
  value zero is given;
begin test: if x < 0 then go to minus else if x < 1 then
        begin integer i ; real y ; array a [1:8] ;
          a [1] := −.57719165 ;
          a [2] := .98820589 ; a [3] := −.89705694 ;
          a [4] := .91820686 ;
          a [5] := −.75670408 ; a [6] := .48219939 ;
          a [7] := −.19352782 ;
          a [8] := .03586834 ; y := a [1];
        for i := 2 step 1 until 8 do y := y × x + a [i] ;
        Gamma := y end hastings
        else Gamma := x × Gamma (x−1) ; go to endgam;
        minus: if x = −1 then Gamma := 0 else
        Gamma := Gamma (x+1) / x ;
        endgam : end gam
```

REMARK ON ALGORITHM 34
GAMMA FUNCTION [M. F. Lipp, *Comm. ACM 4* (Feb. 1961)]
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Computer Applications, Inc., San Diego, Calif.

The coefficients used in the calculation of the Hasting's polynomial are used in reverse order. The algorithm should have
a[1]=−.19352782; a[2]=.48219939; a[3]=−.75670408;
a[4]=.91820686; a[5]=−.89705694; a[6]=.98820589;
a[7]=−.57719165; a[8]=1.0;
y=.03586834;
for i := 1 **step** 1 **until** 8 **do** y := y×x+a[i];.

Further, since Gamma $(x)=\Gamma(1+x)$, the divisor x in the statement labeled minus should be $x+1$.

REMARKS ON:
ALGORITHM 34 [S14]
GAMMA FUNCTION
[M. F. Lipp, *Comm. ACM 4* (Feb. 1961), 106]
ALGORITHM 54 [S14]
GAMMA FUNCTION FOR RANGE 1 TO 2
[John R. Herndon, *Comm. ACM 4* (Apr. 1961), 180]
ALGORITHM 80 [S14]
RECIPROCAL GAMMA FUNCTION OF REAL ARGUMENT
[William Holsten, *Comm. ACM 5* (Mar. 1962), 166]
ALGORITHM 221 [S14]
GAMMA FUNCTION
[Walter Gautschi, *Comm. ACM 7* (Mar. 1964), 143]
ALGORITHM 291 [S14]
LOGARITHM OF GAMMA FUNCTION
[M. C. Pike and I. D. Hill, *Comm. ACM 9* (Sept. 1966), 684]
M. C. PIKE AND I. D. HILL (Recd. 12 Jan. 1966)
Medical Research Council's Statistical Research Unit, University College Hospital Medical School, London, England

Algorithms 34 and 54 both use the same Hastings approximation, accurate to about 7 decimal places. Of these two, Algorithm 54 is to be preferred on grounds of speed.

Algorithm 80 has the following errors:
(1) *RGAM* should be in the parameter list of *RGR*.
(2) The lines
if $x = 0$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x = 1$ **then begin** *RGR* := 1; **go to** *EXIT* **end**
should each be followed either by a semicolon or preferably by an **else**.
(3) The lines
if $x = 1$ **then begin** *RGR* := $1/y$; **go to** *EXIT* **end**
and
if $x < -1$ **then begin** $y := y \times x$; **go to** *CC* **end**
should each be followed by a semicolon.
(4) The lines
BB: **if** $x = -1$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x > -1$ **then begin** *RGR* := *RGAM*(x); **go to** *EXIT* **end**
should be separated either by **else** or by a semicolon and this second line needs terminating with a semicolon.
(5) The declarations of **integer** *i* and **real array** *B*[0:13] in *RGAM* are in the wrong place; they should come immediately after
begin real *z*;

With these modifications (and the replacement of the array *B* in *RGAM* by the obvious nested multiplication) Algorithm 80 ran successfully on the ICT Atlas computer with the ICT Atlas ALGOL compiler and gave answers correct to 10 significant digits.

Algorithms 80, 221 and 291 all work to an accuracy of about 10 decimal places and to evaluate the gamma function it is therefore on grounds of speed that a choice should be made between them. Algorithms 80 and 221 take virtually the same amount of computing time, being twice as fast as 291 at $x = 1$, but this advantage decreases steadily with increasing x so that at $x = 7$ the speeds are about equal and then from this point on 291 is faster—taking only about a third of the time at $x = 25$ and about a tenth of the time at $x = 78$. These timings include taking the exponential of *log-gamma*.

For many applications a ratio of gamma functions is required (e.g. binomial coefficients, incomplete beta function ratio) and the use of algorithm 291 allows such a ratio to be calculated for much larger arguments without overflow difficulties.

ALGORITHM 35
SIEVE
T. C. Wood
RCA Digital Computation and Simulation Group, Moorestown, New Jersey

```
procedure  Sieve (Nmax) Primes: (p) ;
           integer Nmax; integer array p ;
comment    Sieve uses the Sieve of Eratosthenes to find all prime
             numbers not greater than a stated integer Nmax
             and stores them in array p. This array should be
             of dimension 1 by entier (2 × Nmax/ℓn (Nmax)) ;
begin integer n, i, j ;
           p[1] := 1 ; p[2] := 2 ; p[3] := j := 3 ;
           for n := 3 step 2 until Nmax do
begin      i := 3 ;
           L1: go to if p[i] ≤ sqrt (n) then a1 else a2 ;
           a1: go to if n/p[i] = n ÷ p[i] then b1 else b2 ;
           b2: i := i + 1 ; go to L1 ;
           a2 : p[j] := n ; j := j + 1 ;
           b1: end end
```

CERTIFICATION OF ALGORITHM 35
SIEVE (T. C. Wood, *Comm. ACM*, March 1961)
P. J. Brown
University of North Carolina, Chapel Hill, N. C.

SIEVE was transliterated into GAT for the Univac 1105 and successfully run for a number of cases.

The statement:

go to if n/p[i] = n ÷ p[i] **then** b1 **else** b2;

was changed to the statement:

go to if n/p[i] − n ÷ p[i] < .5/Nmax **then** b1 **else** b2;

Roundoff error might lead to the former giving undesired results.

CERTIFICATION OF ALGORITHM 35
SIEVE [T. C. Wood, *Comm. ACM*. Mar. 1961]
J. S. Hillmore
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The statement:

go to if $n/p[i] = n \div p[i]$ **then** $b1$ **else** $b2$;

was changed to the statement:

go to if $(n \div p[i]) \times p[i] = n$ **then** $b1$ **else** $b2$;

This avoids any inaccuracy that might result from introducing real arithmetic into the evaluation of the relation.

The modified algorithm was successfully run using the Elliott Algol translator on the National-Elliott 803.

REMARKS ON:

ALGORITHM 35 [A1]
SIEVE [T. C. Wood, *Comm. ACM 4* (Mar. 1961), 151]
ALGORITHM 310 [A1]
PRIME NUMBER GENERATOR 1 [B. A. Chartres, *Comm. ACM 10* (Sept. 1967), 569]
ALGORITHM 311 [A1]
PRIME NUMBER GENERATOR 2 [B. A. Chartres, *Comm. ACM 10* (Sept. 1967), 570]

B. A. Chartres (Recd. 13 Apr. 1967)
Computer Science Center, University of Virginia, Charlottesville, Virginia

The three procedures *Sieve*(m,p), *sieve*1(m,p), and *sieve*2(m,p), which all perform the same operation of putting the primes less than or equal to m into the array p, were tested and compared for speed on the Burroughs B5500 at the University of Virginia. The modification of *Sieve* suggested by J. S. Hillmore [*Comm. ACM 5* (Aug. 1962), 438] was used. It was also found that *Sieve* could be speeded up by a factor of 1.95 by avoiding the repeated evaluation of *sqrt*(n). The modification required consisted of declaring an integer variable s, inserting the statement $s :=$ *sqrt*(n) immediately after $i := 3$, and replacing $p[i] \leq$ *sqrt*(n) by $p[i] \leq s$.

The running times for the computation of the first 10,000 primes were:

Sieve (Algorithm 35)	845 sec
Sieve (modified)	434 sec
*sieve*1	220 sec
*sieve*2	91 sec

The time required to compute the first k primes was found to be, for each algorithm, remarkably accurately represented by a power law throughout the range $500 \leq k \leq 50{,}000$. The running time of *Sieve* varied as $k^{1.40}$, that of *sieve*1 as $k^{1.53}$, and that of *sieve*2 as $k^{1.35}$. Thus the speed advantage of *sieve*2 over the other algorithms increases with increasing k. However, it should be noted that *sieve*2 took approximately 33 minutes to find the first 100,000 primes, and, if the power law can be trusted for extrapolation past this point (there is no reason known why it should be), it would take about 12 hours to find the first million primes.

ALGORITHM 36
TCHEBYCHEFF
A. J. GIANNI
RCA Digital Computation and Simulation Group, Moorestown, New Jersey

```
procedure  tchebycheff (t, x, m, ℓ)  ;
real array  t, x  ;  integer ℓ, m  ;
comment  given a set of m+1 values of x stored in a one-
           dimensional array whose subscripts run from 0
           thru m at least, construct a table of tn(x), n =
           0, 1, ···,ℓ and store it in the two-dimensional
           array t, where you find tn(x[m]) as t[n, m]  ;
begin integer i, k, n  ;
          for k := 0 step 1 until m do begin t[0, k] := 1  ;
          t[1, k] := x[k] end  ;
          for  n := 2 step 1 until ℓ do for i = 0  step  1
            until m do
          t[n,  i] := 2 × x[i] × t[n − 1, i] − t[n − 2,  i]
end  tcheby
```

ALGORITHM 37
TELESCOPE 1

K. A. BRONS
RCA Advanced Programming Group, Pennsauken, N. J.

```
procedure Telescope 1 (N, L, eps, limit, c) ; value limit, L ;
          integer N ; real L, eps, limit ; array c ;
comment: Telescope 1 takes an Nth degree polynomial approxi-
         mation sum_{k=0}^{N} c_k x^k to a function which was valid to
         within eps ≥ 0 over an interval (0, L) and reduces
         it, if possible, to a polynomial of lower degree,
         valid to within limit > 0. The initial coefficients
         c_k are replaced by the final coefficients, and the
         deleted coefficients are replaced by zero. The ini-
         tial eps is replaced by the final bound on the error.
         N is replaced by the degree of the reduced poly-
         nomial. N and eps must be variables.
         This procedure computes the coefficients given in
         the Techniques Department of the ACM Com-
         munications, Vol. 1, No. 9, from the recursion
         formula

                a_{k-1} = -a_k · k·L·(2k - 1) / (2(N + k - 1)·(N - k + 1)) ;

         begin integer k ; array d[0:N] ;
start:   if N < 1 then go to exit ; d[N] := -c[N] ;
         for k := N step - 1 until 1 do
         d[k - 1] := -d[k] × L × k × (k - 0.5)/
           ((N + k - 1) × (N - k + 1)) ;
         if eps + abs (d[0]) < limit then
         begin eps := eps + abs (d[0]) ;
         for k := N step - 1 until 0 do c[k] := c[k] + d[k] ;
         N := N - 1 ; go to start end ;
exit:    end
```

CERTIFICATION OF ALGORITHM 37
TELESCOPE 1 [K. A. Brons, *Comm. ACM*, Mar., 1961]

HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of *Telescope 1* was compiled and tested on the LGP-30 using the ALGOL 60 translator system developed by the Dartmouth College Computer Center. No syntactical errors were found, and the program ran satisfactorily. The 10th degree polynomial obtained by truncating the exponential series was telescoped using $\lim_1^1 = .1_{10} - 2$ and $L = 1.0$. The result was $N = 3$, $eps = .2103005_{10} - 3$, and coefficients +.9997892, −.9930727, +.4636493, −.1026781. The error curve for the telescoped polynomial was computed for $x = 0(.02)1.0$. The error extrema were bounded by *eps* to within 0.5%. The discrepancy is within the range of input conversion and round-off error.

CERTIFICATION OF ALGORITHM 37
TELESCOPE 1 [K. A. Brons, *Comm. ACM*, Mar. 1961]

JAMES F. BRIDGES
Michigan State University, East Lansing, Mich.

This procedure was tested on the CDC 160A, using 160A FORTRAN. The 10th degree polynomial obtained by truncating the series exp $(-x)$ was telescoped using $L = 1$ and lim = 0.001. The result was $N = 3$, eps = $0.21061862_{10} - 3$ and coefficients +0.99978965, −0.99307236, +0.46364955, −0.10267767. The error curve was computed for $x = 0(0.02)1.0$ and no error exceeded eps, the worst error being 2% of eps less than eps.

This result is in close agreement with that of Henry C. Thatcher, Jr. in his Certification (*Comm. ACM*, Aug. 1962). Mr. Thatcher has pointed out that he inadvertantly referred to the series for exp $(-x)$ as the "exponential series" thereby inferring the positive series exp $(+x)$. There is also a typographical error in his eps. It should be $+0.2103505_{10} - 3$.

ALGORITHM 38
TELESCOPE 2

K. A. BRONS
RCA Advanced Programming, Pennsauken, N. J.

```
procedure Telescope 2 (N, L, eps, limit, c) ; value limit, L ;
          integer N ; real L, eps, limit ; array c ;
comment   Telescope 2 takes an Nth degree polynomial ap-
            proximation  sum_{k=0}^{N} c_k x^k  to a function which was
            valid to within eps >= 0 over an interval (-L, L)
            and reduces it, if possible, to a polynomial of
            lower degree, valid to within limit >0. The initial
            coefficients c_k are replaced by the final coefficients,
            and deleted coefficients are replaced by zero. The
            initial eps is replaced by the final bound on the
            error, and N is replaced by the degree of the re-
            duced polynomial. N and eps must be variables.
          This procedure computes the coefficients given in
            the Techniques Department of the ACM Com-
            munications, Vol. 1, No. 9, from the recursion
            formula

                a_{k-2} = -a_k * k*L^2*(k - 1) / ((N + k - 2)*(N - k + 2)) ;

          begin integer k ; real s ; array d[0: N] ;
start:    if N < 2 then go to exit ; d[N] := -c[N] ;
          for k := N step - 2 until 2 do
          d[k - 2] := -d[k] x L↑2 x k x (k - 1)/
            ((N + k - 2) x (N - k + 2)) ;
          if (N/2) - entier (N/2) = 0 then s := d[0] else
            s := d[1]/N ;
          if eps + abs(s) < limit then begin
            eps := eps + abs(s) ;
          for k := N step - 2 until 0 do
            c[k] := c[k] + d[k] ;
          N := N - 1 ; go to start end ;
exit:     end
```

CERTIFICATION OF ALGORITHM 38
TELESCOPE 2 [K. A. Brons, *Comm. ACM*, Mar., 1961]

JAMES F. BRIDGES
Michigan State University, East Lansing, Mich.

This procedure was tested on the CDC 160A using 160A FORTRAN. The 10th degree polynomial obtained by truncating the series expansion of exp $(+x)$ was telescoped using $L = 1.0$ and lim = 0.001. The result was $N = 4$, eps = $0.59159949_{10} - 3$ and coefficients +1.0000447, +0.99730758, +0.49919675, +0.17734729, +0.043793910. Errors were calculated for $x = -1.0(0.02)1.0$. The only error to exceed cps was at $x = 1.0$ and was within 0.6% of eps.

ALGORITHM 39
CORRELATION COEFFICIENTS WITH MATRIX MULTIPLICATION

PAPKEN SASSOUNI
Burroughs Corporation, Pasadena, California

```
procedure NORM (x) number of rows: (m) number of columns:
    (n) normalized output: (y) standard deviations:
    (s) ;
value m, n ; integer m, n ; array x, y, s ;
comment Given an observation matrix [x] consisting of ob-
    servations x_ij on a population, NORM will cal-
    culate
```

$$y_{ij} = \frac{x_{ij} - \bar{x}_j}{\sqrt{\sum_{i=1}^{m} (x_{ij} - \bar{x}_j)^2}} \qquad \begin{matrix} \text{for } i = 1, \cdots, m \\ j = 1, \cdots, n \end{matrix}$$

```
    and the standard deviations
```

$$s_j = \sqrt{\frac{\sum_{i=1}^{m} (x_{ij} - \bar{x}_j)^2}{m}}$$

```
    where x̄_j is the mean of observations on the j-th
    factor ;
begin integer i, j ; real r, h, c, b ;
    r := sqrt (m) ; for j := 1 step 1 until n do
1: begin h := 0 ;
    for i := 1 step 1 until m do
    h := h + x[i, j] ; h := h/m ; b := 0 ;
    for i := 1 step 1 until m do
2: begin c := x[i, j] - h ; b := b + c↑2 ; y[i, j] := c
    end 2 ;
    b := sqrt (b) ;
    for i := 1 step 1 until m do
    y[i, j] := y[i, j]/b ; s[j] := b/r
    end 1
    end NORM ;
comment The normalization is now completed, and we are
    ready to compute the correlation matrix ;
procedure TRANSMULT (y) number of rows: (m) number of
    columns: (n) symmetrical square matrix result:
    (z) ;
value m, n ; integer m, n ; array y, z ;
comment This procedure multiplies two matrices, the first
    being the transpose of the second. The result is a
    symmetrical matrix with respect to the main diag-
    onal, therefore only the lower part of it, including
    the main diagonal, is computed. The upper half is
    obtained by equating corresponding elements;
begin integer i, j, k ; real h ;
    for j := 1 step 1 until n do
    for i := j step 1 until n do
begin h := 0 ;
    for k := 1 step 1 until m do
    h := h + y[k, i] × y[k, j] ; z[i, j] := h ;
    if i ≠ j then z[j, i] := h
    end i
    end TRANSMULT. [z] is the square matrix of the
    correlation coefficients of the initial observation
    matrix [x]
```

ALGORITHM 40
CRITICAL PATH SCHEDULING

B. LEAVENWORTH
American Machine & Foundry Co., Greenwich, Conn.

```
procedure CRITICALPATH (n, I, J, DIJ, ES, LS, EF, LF, TF,
          FF) ;
integer n ; integer array I, J, DIJ, ES, LS, EF, LF, TF,
          FF ;
comment: Given the total number of jobs n of a project, the
    vector pair Ik , Jk representing the kth job, which is thought
    of as an arrow connecting event Ik to event Jk(Ik < Jk ,
    k = 1 ··· , n), and a duration vector (DIJ)k , CRITICAL-
    PATH determines the earliest starting time (ES)k , latest
    starting time (LS)k , earliest completion time (EF)k , latest
    completion time (LF)k , the total float (TF)k , and the free
    float (FF)k . I1 must be 1 and the Ik , Jk must be in ascending
    order. For example, if the first three jobs are labelled (1, 2),
    (1, 3), (3, 4), then the I, J vectors are (1, 1, 3) and (2, 3, 4)
    respectively. The critical path is given by each arrow whose
    total float is zero. The following non-local labels are used for
    exits: out1 — Ik not less than Jk ; out2 — Ik out of se-
    quence ; out3 — Ik missing;
begin
    integer k, index, max, min ; integer array ti, te [1:n] ;
    index := 1 ;
    for k := 1 step 1 until n do
    begin
        if I[k] ≧ J[k] then go to out1 ;
        if I[k] < index then go to out2 ;
        if I[k] > index ∧ I[k] ≠ index + 1 then go to out3 ;
        if I[k] = index + 1 then index := I[k] ;
C:  end ;
    for k := 1 step 1 until n do
        ti[k] := te[k] := 0 ;
    for k := 1 step 1 until n do
    begin
        max := ti[I[k]] + DIJ[k] ;
        if ti[J[k]] = 0 ∨ ti[J[k]] < max then
        ti[J[k]] := max ;
A:  end ti ;
        te[J[n]] := ti[J[n]] ;
        for k := n step −1 until 1 do
    begin
        min := te[J[k]] − DIJ[k] ;
        if te[I[k]] = 0 ∨ te[I[k]] > min then
        te[I[k]] := min ;
B:  end te ;
    for k := 1 step 1 until n do
     begin
        ES[k] := ti[I[k]] ;
        LS[k] := te[J[k]] − DIJ[k] ;
        EF[k] := ti[I[k]] + DIJ[k] ;
        LF[k] := te[J[k]] ;
        TF[k] := te[J[k]] − ti[I[k]] − DIJ[k] ;
        FF[k] := ti[J[k]] − ti[I[k]] − DIJ[k]
     end
end CRITICALPATH
```

REFERENCES

(1) JAMES E. KELLEY, JR. AND MORGAN R. WALKER, "Critical-Path Planning and Scheduling," 1959 Proceedings of the Eastern Joint Computer Conference.

(2) M. C. FRISHBERG, "Least Cost Estimating and Scheduling — Scheduling Phase Only," IBM 650 Program Library File No. 10.3.005.

CERTIFICATION OF ALGORITHM 40
CRITICAL PATH SCHEDULING (B. Leavenworth, *Comm. ACM*, Mar. 1961)

NEAL P. ALEXANDER
Union Carbide Olefins Company, South Charleston, West Virginia

The Critical Path Scheduling algorithm was coded in FORTRAN for the IBM 7070. The following changes were made:

(a) ti [k] := te [k] := 0;

should be

ti [k] := 0;
te [k] := 9999;

(b) **if** te [I[k]] = 0 ∨ te [I[k]] > min **then**

should be

if te [I[k]] > min **then**

This change permits a value of 0 to be calculated for te [I[k]] and remain as the minimum value.

In the statement

if ti [J[k]] = 0 ∨ ti [J[k]] < max **then**

the part of the statement "ti [J[k]] = 0" is redundant and can be omitted.

CERTIFICATION OF ALGORITHM 40
CRITICAL PATH SCHEDULING [B. Leavenworth, *Comm. ACM* (Mar. 1961)]

LARS HELLBERG
Facit Electronics AB, Solna, Sweden.

The Critical Path Scheduling algorithm was transliterated into FACIT-ALGOL-1 and tested on the FACIT EDB. The modifications suggested by Alexander [*Comm. ACM* (Sept. 1961)] were included. Results were correct in all tested schedules.

CERTIFICATION OF ALGORITHM 40
CRITICAL PATH SCHEDULING [B. Leavenworth, *Comm. ACM* 4 (Mar. 1961), 152; 4 (Sep. 1961), 392; 5 (Oct. 1962), 513]

IRVIN A. HOFFMAN (Recd 7 Feb. 1964)
Woodward Governor Co., Rockford, Ill.

The Critical Path Scheduling algorithm was coded in FAST for the NCR315. The modifications suggested by Alexander [*Comm. ACM* 4 (Sept. 1961)] were included. Results were correct in all tested cases. However, the example of the *I*, *J* vectors given in

the comment is incorrect, as it would cause the exit $out3 - I_k$ missing.

[EDITOR'S NOTE. There are also two semicolons which should be removed from the comment of Algorithm 40.—G.E.F.]

ALGORITHM 41
EVALUATION OF DETERMINANT

JOSEF G. SOLOMON
RCA Digital Computation and Simulation Group, Moorestown, New Jersey

```
real procedure  Determinant (A,n);
real array      A; integer n;
comment This procedure evaluates a determinant by triangularization;
begin real      Product, Factor, Temp; array B[1 : n, 1 : n],
                  C[1 : n, 1 : n];
integer         Count, Sign, i, j, r, y;
                Sign := 1; Product := 1;
for             i := 1 step 1 until n do for j := 1 step 1 until
                  n do
begin           B[i,j] := A[i,j]; C[i,j] := A[i,j] end;
for             r := 1 step 1 until n-1 do
begin           Count := r-1;
    zerocheck:  if B[r,r] ≠ 0 then go to resume;
                if Count < n-1 then Count := Count + 1
                else go to zero;
for             y := r step 1 until n do
begin           Temp := B[Count+1,y]; B[Count+1,y] :=
                  B[Count,y]; B[Count,y] := Temp end;
                Sign := - Sign; go to zerocheck;
        zero:   Determinant := 0; go to return;
      resume:   for i := r+1 step 1 until n do
begin           Factor := C[i,r] / C[r,r];
                for j := r+1 step 1 until n do
begin           B[i,j] := B[i,j] - Factor × C [r,j] end end;
for             i := r+1 step 1 until n do
                for j := r+1 step 1 until n do C[i,j] := B[i,j]
                  end;
for             i := 1 step 1 until n do Product := Product
                  × B[i,i]; Determinant := Sign × Product;
      return:   end
```

ALGORITHM 41, REVISION
EVALUATION OF DETERMINANT [Josef G. Solomon, RCA Digital Computation and Simulation Group, Moorestown, N. J.]

BRUCE H. FREED
Dartmouth College, Hanover, N. H.

```
real procedure determinant (a,n);
real array a; integer n; value a,n;
comment This procedure evaluates a determinant by triangularization;
begin real product, factor, temp;
array b[1:n,1:n];
integer count, ssign, i, j, r, y;
ssign := product := 1;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
b[i,j] := a[i,j];
for r := 1 step 1 until n-1 do
begin count := r-1;
zerocheck: if b[r,r] ≠ 0 then go to resume;
if count < n-1 then count := count +1 else go to zero;
for y := r step 1 until n do
begin temp := b[count+1,y];
  b[count+1,y] := b[count,y];
  b[count,y] := temp end;
ssign := -ssign;
go to zerocheck;
zero: determinant := 0; go to return;
resume: for i := r+1 step 1 until n do
begin factor := b[i,r]/b[r,r];
for j := r+1 step 1 until n do
b[i,j] := b[i,j] - factor × b[r,j] end end;
for i := 1 step 1 until n do
product := product × b[i,i];
determinant := ssign × product;
return: end
```

CERTIFICATION OF ALGORITHM 41
EVALUATION OF DETERMINANT [Josef G. Solomon, RCA Digital Computation and Simulation Group, Moorestown, N. J.]

BRUCE H. FREED
Dartmouth College, Hanover, N. H.

When Algorithm 41 was translated into SCALP for running on the LGP-30, the following corrections were found necessary:

1. In the "*y*" loop after "*B[Count,y] := Temp*" and before the "**end**" insert
   "*Temp := C[Count+1,y];*
   C[Count +1,y] := C[Count,y];
   C[Count,y] := Temp"
2. "Sign" is an ALGOL word when uncapitalized. However, many systems (if not all) do not recognize the difference between small and capital letters. For this reason "*Sign*" was changed to "*ssign*" for the LGP-30 run (and in the revision which follows later).

The following addition might be made in the specification as a concession to efficiency: "**value** *A,n;*".

The following changes might be made to make the Algorithm less wordy:

1. for "*Ssign := 1; Product := 1;*"
   put "*Ssign := Product := 1;*"
2. for "**begin** *B[i,j] := A[i,j]; C[i,j] := A[i,j]* **end**;"
   put "*B[i,j] := C[i,j] := A[i,j];*"
3. for "**begin** *B[i,j] := B[i,j] - Factor × C[r,j]* **end end**;"
   put "*B[i,j] := B[i,j] - Factor × C[r,j]* **end**;"

The above corrections and changes were made and the program was run with the correct results, as follows:

$$A = \begin{pmatrix} 10.96597 & 35.10765 & 96.72356 \\ 2.35765 & -84.11256 & .87932 \\ 18.24689 & 22.13579 & 1.11123 \end{pmatrix}$$

Determinant = $.1527313_{10}06$

Hand calculation on a desk calculator gives the value of the determinant for the above matrix as 152,731.3600.

$$A = \begin{pmatrix} 1.0 & 3.0 & 3.0 & 1.0 \\ 1.0 & 4.0 & 6.0 & 4.0 \\ 1.0 & 5.0 & 10.0 & 10.0 \\ 1.0 & 6.0 & 15.0 & 20.0 \end{pmatrix} \quad \text{Determinant} = .9999999_{10}+00$$

The above matrix, being a finite segment of Pascal's triangle, has determinant equal to 1.000000000.

$$A = \begin{pmatrix} 0.0 & 0.0 & 0.0 \\ 5.0 & 9.0 & 2.0 \\ 7.0 & 5.0 & 4.0 \end{pmatrix} \quad \text{Determinant} = .0000000_{10}+00$$

This is, of course, exactly correct.

Finally, one major change can be made which does away with several instructions and reduces variable storage requirements by n^2. This change is the complete removal of matrix C from the program. It is extraneous.

The revised Algorithm was translated into SCALP and run on the LGP-30 with exactly the same results as above.

The revised Algorithm 41 follows.

REMARK ON REVISION OF ALGORITHM 41 EVALUATION OF DETERMINANT [Josef G. Solomon, *Comm. ACM 4* (Apr. 1961), 176; Bruce H. Freed, *Comm. ACM 6* (Sept. 1963), 520]

LEO J. ROTENBERG (Recd 7 Oct. 63)
Box 2400, 362 Memorial Dr., Cambridge, Mass.

While desk-checking the program an error was found. For example, the algorithm as published would have calculated the value zero as the determinant of the matrix

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

The error lies in the search for a nonzero element in the rth column of the matrix b.

Editor's Note. Apparently the best general determinant evaluators in this section are imbedded in the linear equation solvers Algorithm 43 [*Comm. ACM 4* (Apr. 1961), 176, 182; and *6* (Aug. 1963), 445] and Algorithm 135 [*Comm. ACM 5* (Nov. 1962), 553, 557]. They search each column for the largest pivot in absolute value. Algorithm 41 searches only for a nonzero pivot in each column, and will therefore fail for the matrix

$$\begin{bmatrix} 2^{-t} & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}$$

if $t \gg s$, for a machine with s-bit floating point.

It is hoped that soon a good determinant evaluator will be published to take the place of Algorithm 41.—G. E. F.

CERTIFICATION OF: ALGORITHM 41 [F3] EVALUATION OF DETERMINANT [Josef G. Solomon, *Comm. ACM 4* (Apr. 1961), 171] ALGORITHM 269 [F3] DETERMINANT EVALUATION [Jaroslav Pfann and Josef Straka, *Comm. ACM 8* (Nov. 1965), 668]

A. BERGSON (Recd. 4 Jan. 1966 and 4 Apr. 1966)
Computing Lab., Sunderland Technical College, Sunderland, Co. Durham, England

Algorithms 41 and 269 were coded in 803 ALGOL and run on a National-Elliott 803 (with automatic floating-point unit).

The following changes were made:

(i) **value** n; was added to both Algorithms;

(ii) In Algorithm 269, since procedure *EQUILIBRATE* is only called once, it was not written as a procedure, but actually written into the **procedure** *determinant* body.

The following times were recorded for determinants of order N (excluding input and output), using the same driver program and data.

N	T_1 *Algorithm 41* (minutes)	T_2 *Algorithm 269*
10	0.87	0.78
15	2.77	2.18
20	6.47	4.78
25	12.47	8.99
30	21.37	14.98

From a plot of $\ln(T_1)$ against $\ln(N)$ it was found that

$$T_1 = 0.00104N^{2.92}.$$

Similarly,

$$T_2 = 0.00153N^{2.70}.$$

From a plot of T_1 against T_2, it was found that Algorithm 269 was 30.8 percent faster than Algorithm 41, but Algorithm 41 required less storage.

ALGORITHM 42
INVERT

T. C. Wood
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```
procedure Invert (A) order: (n) Singular: (s) Inverse: (A1);
          array A, A1; integer n,s, value n;
comment This procedure inverts the square matrix A of order
  n by applying a series of elementary row operation to the matrix
  to reduce it to the identity matrix. These operations when
  applied to the identity matrix yield the inverse A1. The case
  of a singular matrix is indicated by the value s := 1;
begin     comment augment matrix A with identity matrix;
          array a[1:n, 1:2 × n]; integer i,j;
          for i := 1 step 1 until n do
          for j := 1 step 1 until 2 × n do
          if j ≦ n then a[i,j] := A[i,j] else
          if j = n+1 then a[i, j] := 1.0 else a [i,j] := 0.0;
          comment begin inversion;
          for i := 1 step 1 until n do
begin     integer k, ℓ, ind; j := ℓ := i; ind := s := 0;
    L1:   if a[ℓ,j] = 0 then
          begin ind := 1; if ℓ < n then begin ℓ := ℓ + 1;
          go to L1 end
                else begin s := 1; go to L2 end
          end;
          if ind = 1 then for k := 1 step 1 until 2 × n do
          begin real temp;
                temp := a[ℓ,k];
                a[ℓ,k] := a [i,k];
                a[i,k] := temp end k loop;
          for k := j step 1 until 2 × n do
              a[i,k] := a[i,k] / a[i,j];
          for ℓ := 1 step 1 until n do
          if ℓ ≠ i then for k := 1 step 1 until 2 × n do
              a[ℓ,k] := a[ℓ,k] − a[i,k] × a[ℓ,j];
          end i loop;
          for i := 1 step 1 until n do
          for j := 1 step 1 until n do
              A1[i,j] := a[i,n+j];
    L2:   end of procedure
```

(b) **for** k := j **step** 1 **until** 2 × n **do**
  a[i, k] := a[i, k]/a[i, j];
should be
for k := 2 × n **step** −1 **until** i **do**
  a[i, k] := a[i, k]/a[i, i];

(c) **if** l ≠ i **then for** k := 1 **step** 1 **until** 2 × n **do**
  a[l, k] := a[l, k] − a[i, k] × a[l, j];
should be
if l ≠ i **then for** k := 2 × n **step** −1 **until** i **do**
  a[l, k] := a[l, k] − a[i, k] × a[l, i];

Given these changes, j becomes superfluous in the second i loop, and the other references to j may be changed to references to i.

INVERT obtained the following results:

The computer inverted a 17-by-17 matrix whose elements were integers less than ten in absolute value. When the matrix and its inverse were multiplied together, the largest nondiagonal element in the product was −.00003. Most nondiagonal elements were less than .00001 in absolute value.

INVERT was tested using finite segments of the Hilbert matrix. The following results were obtained in the 4 × 4 case:

16.005	−120.052	240.125	−140.082
−120.052	1200.584	−2701.407	1680.917
240.126	−2701.411	6483.401	−4202.217
−140.082	1680.920	−4202.219	2801.446

The exact inverse is:

16	−120	240	−140
−120	1200	−2700	1680
240	−2700	6480	−4200
−140	1680	−4200	2800

INVERT was also coded for the LGP-30 in machine language and the 24.1 extended range interpretive system. This system, which uses 30 significant bits for the fraction, obtained the following as the inverse of the 4 × 4 Hilbert matrix:

16.000	−120.001	240.001	−140.001
−120.001	1200.006	−2700.015	1680.010
240.001	−2700.016	6480.037	−4200.024
−140.001	1680.010	−4200.024	2800.016

The program coded in the 24.0 interpretive system successfully inverted a matrix consisting of ones on the minor diagonal and zeros everywhere else.

CERTIFICATION OF ALGORITHM 42
INVERT (T. C. Wood, *Comm. ACM*, Apr., 1961)

Anthony W. Knapp and Paul Shaman
Dartmouth College, Hanover, N. H.

INVERT was hand-coded for the LGP-30 using machine language and the 24.0 floating-point interpretive system, which carries 24 bits of significance for the fractional part of a number and five bits for the exponent. The following changes were found necessary:

(a) **if** j = n+1 **then** a[i, j] := 1.0 **else** a[i, j] := 0.0;
should be
if j = n+i **then** a[i, j] := 1.0 **else** a[i, j] := 0.0;

REMARKS ON ALGORITHM 42
INVERT [T. C. Wood, *Comm. ACM*, Apr. 1961]

P. Naur
Regnecentralen, Copenhagen, Denmark

INVERT cannot be recommended since it does not search for pivot and therefore will give poor accuracy. This is confirmed by the figures quoted by Knapp and Shaman in their certification [*Comm. ACM 4* (Nov. 1961), 498]. The results obtained by them using 30 significant bits for the fraction may be compared directly with those obtained using INVERSION II (Algorithm 120) and gjr with the Gier Algol system (see certification below). Inverting the 4 × 4 segment of the Hilbert matrix, the largest error in any element is found to be:

	Subscripts	*Error*
INVERT (Knapp and Shaman)	3,3	0.037
INVERSION II (see certification of Alg. 120)	3,3	0.0306
gjr (see certification of Alg. 120)	4,3	0.00010

In view of this basic shortcoming of Algorithm 42, it is unnecessary to report on other features of it.

CORRECTION TO EARLIER REMARKS ON ALGORITHM 42 INVERT, ALG. 107 GAUSS'S METHOD, ALG. 120 INVERSION II, AND gjr [P. Naur, *Comm. ACM*, Jan. 1963, 38–40.]

P. NAUR
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George Forsythe, Stanford University, in a private communication has informed me of two major weaknesses in my remarks on the above algorithms:

1) The computed inverses of rounded Hilbert matrices are compared with the exact inverses of unrounded Hilbert matrices, instead of with very accurate inverses of the rounded Hilbert matrices.

2) In criticizing matrix inversion procedures for not searching for pivot, the errors in inverting positive definite matrices cannot be used since pivot searching seems to make little difference with such matrices.

It is therefore clear that although the figures quoted in the earlier certification are correct as they stand, they do not substantiate the claims I have made for them.

To obtain a more valid criterion, without going into the considerable trouble of obtaining the very accurate inverses of the rounded Hilbert matrices, I have multiplied the calculated inverses by the original rounded matrices and compared the results with the unit matrix. The largest deviation was found as follows:

	Maximum deviation from elements of the unit matrix		
Order	*INVERSION II*	*gjr*	*Ratio*
2	$-1.49_{10}-8$	$-1.49_{10}-8$	1.0
3	$-4.77_{10}-7$	$-8.34_{10}-7$	0.57
4	$-9.54_{10}-6$	$-3.43_{10}-5$	0.28
5	$-7.32_{10}-4$	$-4.58_{10}-4$	1.6
6	$-1.61_{10}-2$	$-1.42_{10}-2$	1.1
7	$-5.78_{10}-1$	$-5.47_{10}-1$	1.1
8	$-1.20_{10}-2$	$-1.38_{10}1$	8.7
9	$-4.91_{10}1$	$-2.22_{10}1$	2.2

This criterion supports Forsythe's criticism. In fact, on the basis of this criterion no preference of INVERSION II or *gjr* can be made.

The calculations were made in the GIER ALGOL system, which has floating numbers of 29 significant bits.

ALGORITHM 43
CROUT WITH PIVOTING II

HENRY C. THACHER, JR.*
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```
real procedure INNERPRODUCT (u,v) index : (k) start : (s)
    finish : (f);
value s, f; integer k, s, f; real u, v;
comment INNERPRODUCT forms the sum of u(k) × v(k) for
  k = s, s+1, . . . , f. If s > f, the value of INNERPRODUCT is
  zero. The substitution of a very accurate inner product proce-
  dure would make CROUT more accurate;
comment INNERPRODUCT may be declared in the head of
  any block which includes the block in which CROUT is de-
  clared. It may be used independently for forming the inner
  product of vectors;
begin
        real h;
        h := 0; for k := s step 1 until f do h := h+u × v;
        INNERPRODUCT := h
end     INNERPRODUCT;
procedure CROUT II (A, b, n, y, pivot, det, repeat)
comment This procedure is a revision of Algorithm 16, Crout
  With Pivoting by George E. Forsythe, Comm. ACM 3, (1960)
  507-8. In addition to modifications to improve the running of
  the program, and to conform to proper usage, it provides for
  the computation of the determinant, det, of the matrix A. The
  solution is obtained by Crout's method with row interchanges,
  as formulated in reference [1], for solving Ay = b and transform-
  ing the augmented matrix [A b] into its triangular decomposi-
  tion LU with all L(k,k) = 1. If A is singular we exit to 'singular,'
  a nonlocal label. pivot (k) becomes the current row index of
  the pivot element in the k-th column. Thus enough information
  is preserved for the procedure to process a new right-hand
  side without repeating the triangularization, if the boolean pa-
  rameter repeat is true. The accuracy obtainable from CROUT
  would be much increased by calling CROUT with a more accu-
  rate inner product procedure than INNERPRODUCT.
    The contributions of Michael F. Lipp and George E. Forsythe
  by prepublication review and pointing out several errors are
  gratefully acknowledged;
comment Nonlocal identifiers appearing in this procedure are:
  (1) The nonlocal label 'singular', to which the procedure exits
  if det A=0, and (2) the real procedure 'INNERPRODUCT'
  given above;
        value n; array A, b, y; integer n; integer array
          pivot; real det; Boolean repeat;
begin
        integer k, i, j, imax, p; real TEMP, quot;
        det := 1; if repeat then go to 6;
        for k := 1 step 1 until n do
1:      begin
          TEMP := 0;
          for i := k step 1 until n do
2:        begin
            A[i,k] := A[i,k] − INNERPRODUCT (A[i,p], A[p,k],
              p, 1, k−1);
            if abs(A[i,k]) > TEMP then
3:          begin
              TEMP := abs(A[i, k]); imax := i
            end 3
          end 2;
          pivot [k] := imax;
comment We have found that A[imax, k] is the largest pivot in
  column k. Now we interchange rows k and imax;
          if imax ≠ k then
4:        begin det := − det; for j := 1 step 1 until n do
5:        begin
            TEMP := A[k,j]; A[k,j] := A[imax, j]; A[imax, j]
              := TEMP
          end 5;
          TEMP := b[k]; b[k] := b[imax]; b[imax] := TEMP
          end 4;
          comment The row interchange is done. We proceed
            to the elimination;
            if A[k,k] = 0 then go to singular;
            quot := 1.0/A[k,k];
            for i := k+1 step 1 until n do
            A[i,k] := quot × A[i,k];
            for j := k+1 step 1 until n do
              A[k,j] := A[k,j] − INNERPRODUCT (A[k,p]
                A[p,j], p, 1, k−1);
              b[k] := b[k] − INNERPRODUCT (A[k,p], b[p]
                p, i, k−1)
            end 1; go to 7;
          comment The triangular decomposition is now finished,
            and we skip to the back substitution;
6:        begin comment This section is used when the formal
          parameter repeat is true, indicating that the matrix A
          has previously been decomposed into triangular form by
          CROUT II, with row interchanges specified by pivot,
          and that it is desired to solve the linear system with a
          new vector b, without repeating the triangularization;
            for k := 1 step 1 until n do
            begin
              TEMP := b[pivot[k]]; b[pivot[k]] := b[k]; b[k] :=
                TEMP; b[k] := b[k] − INNERPRODUCT
                (A[k, p], b[p], p, 1, k−1) end;
          end 6;
7:        for k := n step − 1 until 1 do
8:        begin if ¬ repeat then det := A[k,k] × det;
          y[k] := (b[k] − INNERPRODUCT (A[k,p], y[p], p,
            k+1, n)/A[k,k]
          end 8;
end CROUT II;
```

REFERENCE:

(1) J. H. WILKINSON, Theory and practice in linear systems. In John W. Carr III (editor), Application of Advanced Numerical Analysis to Digital Computers, pp. 43-100 (Lectures given at the University of Michigan, Summer 1958, College of Engineering, Engineering Summer Conferences, Ann Arbor, Michigan [1959]).

* Work supported by the U. S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 43
CROUT II (Henry C. Thacher, Jr., *Comm. ACM*, 1960)

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CROUT II was coded by hand for the Royal Precision LGP-30 computer, using a 28-bit mantisa floating point interpretive system (24.2 modified).

The program was tested against the linear system:

$$A = \begin{pmatrix} 12.1719 & 27.3941 & 1.9827 & 7.3757 \\ 8.1163 & 23.3385 & 9.8397 & 4.9474 \\ 3.0706 & 13.5434 & 15.5973 & 7.5172 \\ 3.0581 & 3.1510 & 6.9841 & 13.1984 \end{pmatrix} \quad b = \begin{pmatrix} 6.6355 \\ 6.1304 \\ 4.6921 \\ 2.5393 \end{pmatrix}$$

with the following results:

$$A' = \begin{pmatrix} 12.171900 & 27.394100 & 1.9827000 & 7.3756999 \\ 0.25226957 & 6.6327021 & 15.097125 & 5.6565352 \\ 0.25124262 & -0.56260107 & 14.979620 & 14.527683 \\ 0.66680633 & 0.76468695 & -0.20207132 & -1.3606142 \end{pmatrix}$$

$$b' = \begin{pmatrix} 6.6354999 \\ 3.0181653 \\ 2.5702026 \\ -0.082780734 \end{pmatrix} \quad \text{pivot} = \begin{pmatrix} 1 \\ 3 \\ 4 \\ 4 \end{pmatrix} \quad y = \begin{pmatrix} 0.15929120 \\ 0.14691771 \\ 0.11257482 \\ 0.060840712 \end{pmatrix}$$

det = −1645.4499. All elements of Ab − y were less than 10^{-7} in magnitude. Identical results were obtained with the same b, and repeat **true**. With the same b and the last row vector of A replaced by (19.1927, 33.4409, 25.1298, 5.2811), i.e. A 4, j = A 1 j, + 2A 2, j − 3A 3, j, the results were:

det = $0.10924352 \times 10^{-3}$,

y = (0.29214425×10^{8}, $-0.12131172 \times 10^{8}$, 0.72411923×10^{7}, $-0.51018392 \times 10^{7}$)

Failure to recognize this singular matrix is due to roundoff, either in the data input or in the calculation.

---

* Work supported by the U.S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 43
CROUT II [Henry Thacher, Jr., *Comm. ACM* (1960), 176]

C. DOMINGO AND F. RODRIGUEZ-GIL
Universidad Central, Caracas, Venezuela

CROUT II was coded in PUC-R2 and tested in the IBM-1620. Two types of INNERPRODUCT subroutines were used. The first one finds the scalar product in fixed-point arithmetic to increase accuracy, using an accumulator of 32 digits. The second one uses ordinary floating-point with eight significative figures.

Using a unit matrix as right-hand side, a 6 × 6 segment of Hilbert matrix was inverted. The inverse was inverted again.

The maximum difference between this result and the original segment of Hilbert matrix was:

Using fixed-point INNERPRODUC..... 8.2426×10^{-4}
(Value of determinant..... $4.7737088 \times 10^{-18}$)
Using floating-point INNERPRODUC..... 3.014016×10^{-2}
(Value of determinant..... $4.4950721 \times 10^{-18}$)

Two typographical errors were observed in the algorithm:

The statement:

$$b[k] := g[k] - \text{INNERPRODUCT}\ (A[k,p], b[p], p,i,k-1)$$

should be:

$$b[k] := b[k] - \text{INNERPRODUCT}\ (A[k,p], b[p], 1,k-1)$$

The statement:

$$y[k] := (b[k] - \text{INNERPRODUCT}\ (A[k,p], y[p], p,k+1,n)/A[k,k]$$

should be:

$$y[k] := (b[k] - \text{INNERPRODUCT}\ (A[k,p], y[p], p,k+1,n))/A[k,k]$$

Storage may be saved eliminating the array y and using instead the array b, in which the solution is formed.

A previous certification of this algorithm [*Comm. ACM* 4, 4 (Apr. 1961), 182] was tested again with the same results. Two errors were detected in the certification: The row that must replace the last row of A in order to obtain a singular matrix must be:

19,1927 33.4409 −251298 −5.2811

ALGORITHM 44

BESSEL FUNCTIONS COMPUTED RECURSIVELY

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```
procedure Bessfr(N, FX, LX, Z) Result: (J, Y);
    value LX, FX, N;
    real FX, LX, Z; real array J, Y; integer N;
comment Bessel Functions of the first and second kind, JP(X)
  and YP(X), integral order P, are computed by recursion for
  values of X, FX ≦ X ≦ LX, in steps of Z. The functions are
  computed for values of P, 0 ≦ P ≦ N. M[SUB], the initial
  value of P being chosen according to formulae in Erdelyi's
  Asymptotic Expansions. The computed values of JP(X) and
  YP(X) are stored as column vectors for constant argument in
  matrices J, Y of dimension (N+1) by entier ((LX − FX)/Z + 1);
begin real PI, X, GAMMA, PAR, LAMDA, SUM, SUM1;
    integer P, SUB, MAXSUB;
            PI := 3.14159265;
            GAMMA := .57721566;
            PAR := 63.0 − 1.5 × ℓn (2 × PI);
            MAXSUB := entier ((LX − FX)/Z);
begin real array JHAT [0:N, 0:MAXSUB];
    integer array M[0:MAXSUB];
        SUB := 0;
      for X := FX step Z until LX do
begin if (X > 0) ∧ (X < 10) then M [SUB] := 2 × entier (X) + 9
  else
begin real ALOG;
      ALOG := (PAR − 1.5 × ℓn (X))/X;
      M [SUB] := entier (X × (exp (ALOG) + exp
        (−ALOG))/2) end;
      if N > M [SUB] then
begin for P := M [SUB] + 1 step 1 until N do
      J [P, SUB] := 0 end;
      JHAT [M [SUB], SUB] := 10 ↑ (−9);
comment Having set the uppermost ĴP(X) to a very small
  number we are now going to compute all the ĴP(X) down to
  P = 0;
    for P := M [SUB] step −1 until 1 do
    JHAT [P−1, SUB] := 2 × P/X × JHAT [P, SUB] −JHAT
      [P+1, SUB];
    SUM := SUM1 := 0;
    for P := 2 step 2 until (M [SUB] ÷ 2) do
    SUM := SUM + JHAT [P, SUB];
    LAMDA := JHAT [0, SUB] + 2 × SUM;
    for P := 0 step 1 until N do
    J [P, SUB] := JHAT [P, SUB] /LAMDA;
comment JP(X) have been computed by use of ĴP(X);
    for P := 2 step 2 until (M [SUB] ÷ 2) do
    SUM1 := SUM1 + (−1) × (−1) ↑ P ÷ J [2 × P, SUB]
      /2/P;
    Y [0, SUB] := 2/PI × (J [0, SUB] × (GAMMA + ℓn(X/2))
      + 4 × SUM1);
    for P := 0 step 1 until (M[SUB]−1) do
    Y [P+1, SUB] := (−2/PI/P + J [P+1, SUB] × Y [P,
      SUB])/J [P, SUB];
    SUB := SUB + 1 end end end
```

ALGORITHM 45
INTEREST

PETER Z. INGERMAN
University of Pennsylvania, Philadelphia, Pa.

```
procedure monpay (i, B, L, t, k, m, tol, goof)
comment This procedure calculates the periodic payment
  necessary to retire a loan when the interest rate on the loan
  varies (possibly from period to period) as a function of the as-
  yet-unpaid principal.
    The formal parameters are: i, array identifier for the vector
  of interest rates; −B, array identifier for the minimum amounts
  at which the corresponding i applies; −L, the amount to be
  borrowed; −t, the number of periods for which the loan is to
  be taken out; −k, the number of different interest rates (and
  upper limit for vectors i and B); −m, the desired periodic pay-
  ment; −tol, the allowable deviation of m from some ideal;
  and goof, the error exit to use if convergence fails. The only
  output parameter is m. For further discussion, see Comm.
  ACM 3 (Oct. 1960), 542;
begin array h, S [1:k, 1:t], M, X [1:k];
integer array T, a, b [1:k];
integer p, q, r, sa, sb, I, ib, mb, nb;
comment This section sets up the procedure;
for p := 1 step 1 until k do
begin for q := 1 step 1 until t do
    begin h[p,q] := i[p]↑q;
          S[p,q] := (h[p,q] − 1)/(i[p] − 1) end;
    if p = 1 then X[p] := 0 else X[p] := B[p] × (i[p−1] − i[p]);
    M[p] := L × (h[p,t]/S[p,t]) end;
sa := sb := ib := mb := 0; nb := t;
for p := 1 step 1 until k do
begin a[p] := entier (B[p+1]/M[p+1] + 0.5) − sa;
      sa := sa + a[p];
      T[p] := b[p] := entier (B[p+1]/M[p] − 0.5) − sb;
      sb := sb + b[p];
      if b[p] > mb then
      begin ib := p; nb := nb − mb; mb := bp end
      else nb := nb − b[p] end;
T[ib] := nb;
I := 1;
for p := 1 step 1 until k do
    I := I × (a[p] − b[p] + 1);
comment Having counted the number of possible iterations
  and established a set of trial values for the T[n]'s, a trial m is
  found;
D := 1; E := F := 0;
newm: for p := 1 step 1 until k do
      begin D := D × h[p,Tp];
            u := 1;
            if p ≠ 1 then for q := 1 step 1 until p − 1
              do u := u × h[q,Tq];
            E := E + S[p,Tp] × u;
            v := 0;
            if p ≠ 1 then for r := 1 step 1 until p
              do v := v + X[r];
            F := F + u × v end;
      m := (L × D + F)/E;
      comment Now find out whether m is good enough
      q := 1; F := D := 0;
      for p := 1 step 1 until t do
      begin get F: F := (D + m − E)/(1 + i[q]);
            if B[q+1] ≧ F then D := F else q := q + 1;
            if D ≠ F go to get F end;
            if abs (D − L) ≦ tol then go to exit;
      comment If not within tolerance, adjust T[n]'s and try
        again;
      p := 0;
      redo: p := p + 1;
          if p ≠ ib then
          begin if T[p] ≧ a[p] then
                begin T[ib] := T[ib] + T[p] − b[p]
                      T[p] := b[p] end end
          else begin
              T[p] := T[p] + 1;
              T[ib] := T[ib] − 1;
              p := k end;
          if p = k then I := I − 1 else go to redo;
          go to if I > 0 then newm else goof;
exit: end monpay;
```

CERTIFICATION OF ALGORITHM 45
INTEREST [Peter Z. Ingerman, *Comm. ACM* Apr. 1961 and Oct. 1960]

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INTEREST was translated into Dartmouth College Computation Center's "Self Contained ALGOL Processor" for the Royal-McBee LGP-30. When using SCALP, memory capacity is severely limited and thus it was necessary to run this program in two blocks. Block I ended with the computation of I, and Block II started with the "*newm*" loop. After making the changes listed below, test problems using up to three interest rates and up to 18 time periods were used with the following results:

Loan	*Periods*	*Interest Rates*	*Payments*	*Final Balance**	*Tolerance*
$100.00	1	0.05	$105.00	$0.00	$0.25
1800.00	10	0.03	211.01	0.05	4.50
875.65	8	0.08 to 500.00			
		0.05 over 500.00	139.78	−1.49	2.19
14750.00	18	0.06 to 5000.00			
		0.05 to 10,000.00			
		0.04 over 10,000.00	1201.70	10.55	36.88

* Hand calculation.

It is noted that in each case the final balance is within the prescribed tolerance (0.0025 of the loan).

In the following corrections bracketed subscripts replace ordinary subscripts and exponentiation is represented by ↑ rather than superscript.

The following corrections should be made in the Note on Interest in the October, 1960, issue of *Comm. ACM*:

1. Definition of $B[n]$: Replace "*minimum*" by "*maximum*". Replace "$j[n]$" by "$j[n-1]$".
2. Define $B[k+1] \equiv L$.
3. Definition of $K[n]$: Replace "$B[n]$" by "$B[n+1]$".

The following corrections were found necessary in the procedure:

1. The upper limit of the vector B is $k+1$, not k. It is not necessary to change the upper limit of the I-vector. (See correction 4 below.)

2. D, E, F, u, v were not declared and must be declared as **real**.

3. In the **array** declaration replace "$M[1:k]$" by "$M[1:k+1]$".

4. As j approaches 0, i approaches 1 and $\lim (h/S) = 1/t$. Thus for $j[k+1] = 0$, $i[k+1] = 1$, and $M[k+1] = L/t$. Thus after

$M[p] := L \times (h[p,t]/S[p,t])$ **end**;

insert

$M[k+1] := L/t$; $B[k+1] := L$;

5. In the conditional statement following computation of $b[p]$, replace "$>$" by "$\geqq$".

6. In same conditional statement, next line, "$mb := bp$" should read "$mb := b[p]$".

7. $D := 1$; $E := F := 0$;

newm: for $p := 1$ **step** 1 **until** k **do**

should be changed to

newm: $D := 1$; $E := F := 0$;

for $p := 1$ **step** 1 **until** k **do**

8. **begin** *get F*: $F := (D+m-E)/(1+i[q])$;

if $B[q+1] \geqq F$ **then** $D := F$ **else** $q := q + 1$;

if $D \neq F$ **go to** *get F* **end**;

should be changed to read as follows:

begin *get F*: $F := (D+m)/i[q]$;

if $B[q+1] \geqq F$ **then** $D := F$ **else**

begin if $q < k$ **then** $q := q + 1$ **else** $D := F$ **end**;

if $D \neq F$ **then go to** *get F* **end**;

Note that the "then" in the last line was omitted from the original procedure.

9. In the "*redo*" loop insert a semicolon after the statement

$T[ib] := T[ib] + T[p] - b[p]$;

10. In the "*redo*" loop, next line, omit the second "*end*".

11. In the "*redo*" loop,

$p := k$ **end**;

should be changed to

$p := k$ **end end**;

ALGORITHM 46
EXPONENTIAL OF A COMPLEX NUMBER
JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure EXPC (a, b, c, d); value a, b; real a, b, c, d;
comment This procedure computes the number, c+di, which
  is equal to e^(a+bi);
begin  c := exp (a);
       d := c × sin (b);
       c := c × cos (b)
end EXPC;
```

CERTIFICATION OF ALGORITHM 46
EXPONENTIAL OF A COMPLEX NUMBER (J. R. Herndon, *Comm. ACM 4* (Apr., 1961), 178)
A. P. RELPH
Atomic Power Div., The English Electric Co., Whetstone, England

Algorithm 46 was translated using the DEUCE ALGOL compiler, no corrections being required, and gave satisfactory results.

ALGORITHM 47
ASSOCIATED LEGENDRE FUNCTIONS OF THE FIRST KIND FOR REAL OR IMAGINARY ARGUMENTS

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure LEGENDREA (m, n, x, r); value m, n, x, r;
          integer m, n; real x, r;
comment This procedure computes any P_n^m(x) or P_n^m(ix) for
  n an integer less than 20 and m an integer no larger than n.
  The upper limit of 20 was taken because (42)! is larger than
  10^49. Using a modification of this procedure values up to n=35
  have been calculated. If P_n^m(x) is desired, r is set to zero. If
  r is nonzero, P_n^m(ix) is computed;
begin
          integer i, j; array Gamma [1:41];
          real p, z, w, y;
          if n = 0 then
            begin p := 1;
            go to gate end;
          if n < m then
            begin p := 0;
            go to gate end;
          z := 1; w := z;
          if n=m then go to main;
          for i := 1 step 1 until n-m do
            z := x × z;
    main: Gamma [1] := 1;
          for i := 2 step 1 until n+n+1 do
            begin Gamma [i] := w × Gamma [i-1];
            w := w+1 end;
          w := 1;  y := w/(x × x);
          if r=0 then
            begin y := -y;
            w := -w end;
          if x=0 then
            begin i := (n-m)/2;
            if (i+i) ≠ (n-m) then
              begin p := 0;
              go to gate end;
            p := Gamma [m+n+1]/(Gamma [i+1] × Gamma
              [m+i+1]);
            go to last end;
          j := 3;  p := 0;
          for i := 1 step 1 until 12 do
            begin if (n-m+2)/2 < i then go to last end;
            p := p + Gamma [n+n-i-i+3] × z/(Gamma
              [i] × Gamma [n-i+2] × Gamma [n-i-i-
              m+j]);
            z := z × y end;
    last: z := 1;
          for i := step 1 until n do
            z := z+z;
          p := p/z;
          if r ≠ 0 then
            begin i := n-n/4;
            if 1 < i then
              p := -p end;
          if m = 0 then go to gate;
          j := m/2;  z := abs(w+x × x);
          if m ≠ (j+j) then
            begin z := sqrt (z);
            j := m end;
          for i := step 1 until j do
            p := p × z;
    gate: LEGENDREA := p
end LEGENDREA;
```

CERTIFICATION OF ALGORITHM 47
ASSOCIATED LEGENDRE FUNCTIONS OF THE FIRST KIND FOR REAL OR IMAGINARY ARGUMENTS [John R. Herndon, *Comm. ACM*, Apr. 1961]

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* Work supported by United States Atomic Energy Commission.

This procedure was programmed in FORTRAN for the IBM 1620 and was tested with a number of real arguments. A few errors were detected:

1. In the following sequence the *end* must be removed:

   begin if $(n - m + 2)/2 < i$ **then go to last end**;

2. In these, the lower bound of 1 is needed:

   for i := **step** 1 **until** n **do**
   for i := **step** 1 **until** j **do**

3. There are four places where integer arithmetic is clearly intended and we must substitute the symbol ÷ for the symbol /.

In addition, it might be mentioned that the statement

if $n = m$ **then go to** main;

could be omitted from the ALGOL program without harm, though the FORTRAN version requires it. Here, and elsewhere in the procedure, one might make an equivalent but more succinct statement. With change in style, the variable j could be eliminated.

CERTIFICATION OF ALGORITHM 47 [S16]
ASSOCIATED LEGENDRE FUNCTIONS OF THE FIRST KIND FOR REAL OR IMAGINARY ARGUMENTS [John R. Herndon, *Comm. ACM 4* (Apr. 1961), 178]

S. M. COBB (Recd. 6 Feb. 1969, 12 May 1969 and 9 July 1969)
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KEYWORDS AND PHRASES: Legendre function, associated Legendre function, real or imaginary arguments
CR CATEGORIES: 5.12

This procedure was tested and run on the I.C.T. Atlas computer.

In addition to the errors mentioned in the certification of August 1963 [2] the following points were noted.

1. The requirement that when $n < m$ $p := 0$ must take precedence over $p := 1$ when $n = 0$. Hence the order of the first two **if** statements must be interchanged.

2. Most computers fail on division by zero. Hence the statement beginning **if** $x = 0$ **then** and ending with **go to** *last* **end**; should be inserted between $w := 1$; and $y := w/(x \times x)$.

3. When $x = 0$, if the argument of the Legendre function is to be considered as real p must be multiplied by $(-1)^i$. This is achieved by inserting after the statement beginning $p :=$ *Gamma*$[m+n+1]$ the **if** statement

if r **then** $p := p \times (-1) \uparrow i$;

(For a change in the meaning of r see item 5 below.)

4. After the label *last* in the compound statement beginning **if** $r \neq 0$ the statement $i := n - n \div 4$; is wrong. This should read

$i := n - 4 \times (n \div 4)$;

5. Since r is used only as an indicator it is better that it be declared as **Boolean**. It can then be given the value **true** if the argument of the Legendre function is x and **false** if it is ix. The following program changes are then necessary. The statement beginning

if $r = 0$ **then**

becomes

if r **then**

The statement beginning

if $r \neq 0$ **then**

becomes

if $\neg r$ **then**

6. Computing time can be saved in several ways. First we should declare another integer k and set it equal to $n - m$. The first statement of the procedure is then

$k := n - m$;

The next statement will begin

if $k < 0$ **then**

(This replaces **if** $n < m$ **then** whose position has been changed in accordance with item 1 above.)
$n - m$ is then replaced by k in the lines
for $i := 1$ **step** 1 **until** $n - m$ **do**

and

if $(i+1) \neq (n-m)$ **then**

Removing j as suggested in the previous certification leaves it free to be set to $k \div 2$. This requires the following modification: instead of the unnecessary statement **if** $n = m$ **then go to** *main* put

$j := k \div 2$;

In the statement beginning **if** $x = 0$ **then** replace the line

begin $i := (n-m) \div 2$;

by

begin $i := j$;

In the **for** loop beginning **for** $i := 1$ **step** 1 **until** 12 **do** a further small saving in computer time could be achieved by setting k to $n - i$. The loop thus becomes

for $i := 1$ **step** 1 **until** 12 **do**
begin if $j + 1 < i$ **then go to** *last;*
$k := n - i$;
$p := p +$ *Gamma*$[2 \times k+3] \times z/$*Gamma*$[i] \times$ *Gamma*$[k+2] \times$ *Gamma*$[k-i-m+3])$;
$z := z \times y$
end

For real argument the program was tested as follows.

(i) $x = 0(0.1)1$, $m = 0(1)3$, $n = 0(1)3$
(ii) $x = 1.2(0.2)2.8$, $m = 0(1)2$, $n = 0(1)2$
(iii) $m = 0$, $n = 9$, $x = 0(0.2)1$, $2(2)10$.

For imaginary argument we used

$x = 0(0.2)2$, $m = 0(1)2$, $n = 0(1)2$.

Checking for real argument was carried out where possible using [1], agreement being obtained in all cases to the maximum number of figures available, which varied between 6 and 8. For all other cases [3] had to be used, giving only a 5 figure check.

REFERENCES:
1. ABRAMOWITZ, M., AND STEGUN, I. A. Handbook of mathematical functions. AMS 55, Nat. Bur. Stand. US Govt. Printing Off., Washington, D.C., 1964.
2. GEORGE, R. Certification of Algorithm 47. *Comm. ACM 6* (Aug. 1963), 446.
3. MORSE, P. M., AND FESBACH, H. *Methods of Theoretical Physics Pt. II.* McGraw Hill, New York, 1953.

ALGORITHM 48
LOGARITHM OF A COMPLEX NUMBER

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```
procedure LOGC(a, b, c, d); value a, b; real a, b, c, d;
comment This procedure computes the number, c+di, which
  is equal to log_e(a+bi);
begin  c := sqrt (a × a + b × b);
       d := arctan (b/a);
       c := log (c);
       if a < 0 then d := d+3.1415927
end LOGC;
```

CERTIFICATION OF ALGORITHM 48
LOGARITHM OF A COMPLEX NUMBER (J. R. Herndon, *Comm. ACM 4* (Apr., 1961), 179)

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Algorithm 48 was translated using the DEUCE ALGOL compiler, after certain modifications had been incorporated, and then gave satisfactory results.

The original version will fail if $a = 0$ when the procedure for arctan is entered. It also assumes that $-\pi/2<d<3\pi/2$, whereas the principal value for logarithm of a complex number assumes $-\pi<d\leqq\pi$.

Incidentally, the ALGOL 60 identifier for natural logarithm is ln, not log.

The modified procedure is as follows:

```
procedure LOGC (a,b,c,d); value a,b; real a,b,c,d;
comment This procedure computes the number c + di which is
  equal to the principal value of log_e (a + bi). If a = 0 then c is
  put equal to −10↑47 which is used to represent "− infinity";
begin integer m,n
  m := sign (a);  n := sign (b);
  if a = 0 then begin c := −10↑47;
                      d := 1.5707963 × n;
                      go to k
  end;
  c := sq rt(a × a + b × b);
  c := ln (c);
  d := 1.5707963 × (1−m) × (1+n−n×n) + arctan (b/a);
k: end LOGC;
```

REMARK ON ALGORITHM 48
LOGARITHM OF A COMPLEX NUMBER [John R. Herndon, *Comm. ACM 4* (Apr. 1961)]

MARGARET L. JOHNSON AND WARD SANGREN
Computer Applications, Inc., San Diego, Calif.

Considerable care must be taken in using the arctan function. In Algorithm 48 two such difficulties are ignored. First it is necessary, because of a resulting division by zero, to deal separately with the case where the real part of the complex number is zero. Second, if the real part of the complex number is negative and the argument of the logarithm is to have a value between $-\pi$ and π then the action depends upon the sign of the imaginary part of the complex number. For clarity the following procedure exhibits in sequence the alternatives:

```
procedure LOGC (a, b, c, d); value a, b; real a, b, c, d;
comment This procedure computes the number c+di which is
  equal to log_e (a+bi). It is assumed that the arctan has a value
  between −π/2 and π/2.
begin  if a>0 then begin THETA := 0;  go to SOL end;
       if a<0∧b≧0 then begin THETA := 3.1415927;
         go to SOL end;
       if a<0∧b<0 then begin THETA := −3.1415927;
         go to SOL end;
       if a=0∧b=0 then begin c := d := 0;
         go to RETURN end;
       if a=0∧b>0 then begin c := ln(b);  d := 1.570963;
         go to RETURN end;
       if a=0∧b<0 then begin c := ln(abs(b));
         d := 1.570963;  go to RETURN end;
 SOL:  d := arctan (b/a) + THETA;
       c := sqrt(a×a+b×b);
       c := ln(c);
RETURN: end LOGC
```

REMARK ON REMARKS ON ALGORITHM 48 [B3]
LOGARITHM OF A COMPLEX NUMBER [John R. Herndon, *Comm. ACM 4* (Apr. 1961), 179; *5* (Jun. 62), 347; *5* (Jul. 62), 391]

DAVID S. COLLENS (Recd. 24 Jan. 1964 and 1 Jun. 1964)
Computer Laboratory, The University, Liverpool 3, England

This procedure was designed to compute $\log_e(a+bi)$, namely $c+di$, and although some very necessary precautions about its use have already been stated, some points seem to have escaped notice. In particular, A. P. Relph [*Comm. ACM*, June 1962, 347] remarked that if $a = 0$, then c becomes '−infinity', but this is only the case if $b = 0$ also. Margaret L. Johnson and Ward Sangren [*Comm. ACM*, July 1962, 391] conceded that $a = b = 0$ was a special case, but wrongly gave zero as the result. The only reasonable way of dealing with this case is to exit to some nonlocal label and to let the user decide whether to terminate his program or to assign particular values to c and d. The obvious values to use here are, for c, a negative number, larger than the largest which would be given by the procedure, and possibly zero for d. (In an implementation where 2^{-129} is the smallest representable nonzero number, the largest negative value of c possible is −89.416.) Finally, in the Johnson-Sangren version of the procedure, the last conditional statement should read

```
if a = 0 ∧ b < 0 then begin c := ln(abs(b));
  d := −1.570963;  go to RETURN end;
```

the omission of the minus sign in the original being probably typographical in origin.

ALGORITHM 49
SPHERICAL NEUMANN FUNCTION
JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
real procedure SPHBEN (r,x); value r,x; real r,x;
comment This procedure computes the spherical Neumann
  function (π/2x)^½ N_{r+1/2}(x). Infinity is represented by 10^47;
begin real z, g, t;
      if x=0 then
        begin s := 10 ↑ 47;
          go to gate
        end;
      s := −cos (x)/x;
      if r = 0 then
        go to gate;
      t := sin (x)/x;
      for g := 1 step 1 until r do
        begin z := s;
          s := s × (g+g−1)/(x−t):
          t := z
        end;
gate: SPHBEN := s
end SPHBEN;
```

ACM Transactions on Mathematical Software, Vol. 4, No. 3, September 1978, Page 295.

REMARK ON ALGORITHM 49

Spherical Neumann Function
[J.R. Herndon, *Comm. ACM 4,* 4 (April 1961), 179]

John P. Coleman [Recd 17 February 1978]
Department of Mathematics, University of Durham, Durham, England

There is a typographical error in this algorithm. The line

$$s := s \times (g + g - 1)/(x - t);$$

should read

$$s := s \times (g + g - 1)/x - t;$$

The algorithm provides overflow protection only when $x = 0$. Overflow will still occur for x very close to zero. The range of values of x for which overflow occurs will depend both on the value of r and on the largest number the machine can hold.

ALGORITHM 50
INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure INVHILBERT (n,S); value n; real n;
          real array S;
comment This procedure computes the elements of the inverse
  of an n × n finite segment of the Hilbert matrix and stores them
  in the array S;
begin     real i, j, k;
          S[1, 1] = n × n;
          for i := 2 step 1 until n do
            begin
              S[i, i] := (n+i−1) × (n−i+1)/((i−1) × (i−1));
              S[i, i] := S[i−1, i−1] × S[i, i] × S[i, i]
            end;
          for i := 1 step 1 until n−1 do
            begin
              for j := i+1 step 1 until n do
                begin
                  k := j−1;
                  S[i, j] := −S[i, k] × (n+k) × (n−k)/(k × k)
                end
            end;
          for i := 2 step 1 until n do
            begin S[i, i] := S[i, i]/(i+i−1);
              for j := 1 step 1 until i−1 do
            begin S[j, i] := S(j, 1]/(i+j−1);
                  S[i, j] := S[j, i]
            end
          end
end INVHILBERT;
```

CERTIFICATION OF ALGORITHM 50
INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX [J. R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

B. RANDELL
Atomic Power Division, The English Electric Co., Whetstone, England

INVHILBERT was translated using the DEUCE ALGOL compiler and the following corrections being needed.

1. S[1, 1] = n × n, replaced by S[1, 1] := n × n;
2. S[j, i] := S(j, 1]/(i + j − 1)
replaced by S[j, i] := S[j, i]/(i + j − 1)

The compiled program, which used a 20 bit mantissa floating point notation then produced the following 4 × 4 segment

16.0	−120.0	240.0002	−140.0
−120.0	1200.0	−2700.0	1680.0019
240.0	−2700.0	6480.0	−4200.0
−140.0	1680.0019	−4200.0	2800.0039

REMARKS ON AND CERTIFICATION OF ALGORTHM 50
INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX [J. R. Herndon, *Comm. ACM*, Apr. 1961]

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In addition to inserting the corrections indicated by B. Randell [*Comm. ACM* 5 (Jan. 1962), 50], we have modified and simplified the algorithm as follows:

1. The types of n, i, j and k have been changed to **integer.** This saves roundoff operations in subscripts.

2. Explicit multiplications have been replaced by squaring. This saves code length and execution time, at least in a compiler like ours for the GIER.

3. Repeated references to subscripted variables have been eliminated, partly with the aid of an additional simple working variable, w, partly by using simultaneous assignments.

4. An unnecessary **begin end** pair has been removed.

In total, these changes, in addition to reducing the code length, have increased speed by a factor of 1.6.

The resulting algorithm is as follows:

```
procedure INVHILBERT(n,S);
value n; integer n; real array S;
comment ALG. 50: This procedure computes the elements of
  the inverse of an n × n finite segment of the Hilbert matrix and
  stores them in the array S. The Hilbert matrix has the elements
  HILBERT[i,j] = 1/(i+j−1). The segments of this are known
  to be increasingly ill-conditioned with increasing size;
begin integer i, j, k; real w;
w := S[1,1] := n↑2;
for i := 2 step 1 until n do w := S[i,i] := w × ((n+i−1) ×
    (n−i+1)/(i−1)↑2)↑2;
for i := 1 step 1 until n−1 do for j := i+1 step 1 until n do
  begin
  k := j−1;
  S[i,j] := −S[i,k] × (n+k) × (n−k)/k↑2
  end;
for i := 2 step 1 until n do for j := 1 step 1 until i do
  S[i,j] := S[j,i] := S[j,i]/(i+j−1)
end INVHILBERT;
```

Both the original version and the above improved one have been run successfully on the GIER ALGOL system (30-bit mantissa). The test program included:

(a) Output of the 4 × 4 matrix, to be compared with the results of Randell [loc. cit.]. Results:

16.000000	−120.000000	240.000000	−140.000000
−120.000000	1200.000000	−2700.000000	1680.000000
240.000000	−2700.000000	6480.000000	−4200.000000
−140.000000	1680.000000	−4200.000000	2799.999977

(b) For n := 1 **step** 1 **until** 15, the inverse of the segment was calculated by INVHILBERT and multiplied by the segment of the Hilbert matrix, and the result was compared with the unit matrix. The maximum error was divided by the largest element of the inverse to form a relative error. Some of the results, which were entirely satisfactory throughout, are given below:

Order	*Element of max error*	*abs (max error)*	*Largest element of INVHILBERT*	*Relative error*
3	$S[3,3]$	$2.38_{10}-7$	$1.92_{10}2$	$1.24_{10}-9$
6	$S[2,4]$	$4.39_{10}-3$	$4.41_{10}6$	$9.96_{10}-10$
9	$S[2,8]$	$1.24_{10}2$	$1.22_{10}11$	$1.01_{10}-9$
12	$S[5,9]$	$1.54_{10}6$	$3.66_{10}15$	$4.21_{10}-10$
15	$S[1,12]$	$1.06_{10}11$	$1.15_{10}20$	$9.22_{10}-10$

(c) The time for a call of the revised INVHILBERT was found as follows:

n	
5	0.2 seconds
10	0.6 "
15	1.3 "

ALGORITHM 51
ADJUST INVERSE OF A MATRIX WHEN AN ELEMENT IS PERTURBED

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure ADJUST (n, d, i, j, A, B); value i, j, n, d;
          integer i, j, n; real d; real array A, B;
comment If the n × n matrix A=M⁻¹ and a change, d, is made
  in the i, j-th element of M this procedure will calculate the
  corrected matrix for M⁻¹ by adjusting matrix A. The adjusted
  matrix is stored in B;
begin     integer r, s;
          real t;
          t := d/(A[j, i] × d+1);
          for r := 1 step 1 until n do
            begin for s := 1 step 1 until n do
              B[r, s] = A[r, s] − t × A[r, i] × Aj, s] end
end ADJUST
```

CERTIFICATION OF ALGORITHM 51
ADJUST INVERSE OF A MATRIX WHEN AN ELEMENT IS PERTURBED [John R. Herndon, *Comm. ACM 4* (Apr. 1961)]

RICHARD GEORGE*
Argonne National Laboratory, Argonne, Ill.

This procedure was programmed in FORTRAN and reduced to machine code mechanically. It was run on the Argonne-built computing machine, GEORGE. A floating-point routine was used which allows maximum accuracy to 31 bits.

The procedure was tested for matrices with n ranging from 2 to 10. For each value of n, there were 20 successive trials; each trial consisted of a random perturbation of a randomly selected element of the matrix M, followed by a use of ADJUST, followed by the matrix multiplication N := B·M. For each trial, the adjustment was evaluated by computing

$$\text{sum} := \left\{\sum_{i=1}^{n}\sum_{j=1}^{n} N[i,j]\right\} - n.$$

For random perturbations between −1.0 and +1.0, the value of sum never exceeded $2.0_{10}-8$.

There are two typographical errors present:

```
B[r,s]=A[r,s]−t×A[r,i]×Aj,s] end
```

should be

```
B[r,s] := A[r,s]−t×A[r,i]×A[j,s] end
```

* Work supported by the U. S. Atomic Energy Commission.

ALGORITHM 52
A SET OF TEST MATRICES

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure TESTMATRIX (n,A); value n; integer n;
          real array A;
comment This procedure places in A an n × n matrix whose
  inverse and eigenvalues are known. The n-th row and the n-th
  column of the inverse are the set: 1, 2, 3, . . . , n. The matrix
  formed by deleting the n-th row and the n-th column of the
  inverse is the identity matrix of order n−1;
begin     integer i, j;
          real t, c, d, f;
          c := t × (t+1) × (t+t−5)/6;
          d := 1/c;
          A[n, n] := −d;
          for i := 1 step 1 until n−1 do
            begin f := i;
              A[i, n] := d × f;
              A[n, i] := A[i, n];
              A[i, i] := d × (c−f × f);
              for j := 1 step 1 until i−1 do
                begin t := j;
                  A[i, j] := −d × f × t;
                  A[j, i] := A[i, j]
                end
            end
end TESTMATRIX;
```

CERTIFICATION OF ALGORITHM 52
A SET OF TEST MATRICES (J. R. Herndon, *Comm. ACM*, Apr. 1961)

H. E. GILBERT
University of California at San Diego, La Jolla, Calif.

The statement

```
c := t × (t+1) × (t+t−5)/6;
```

was changed to

```
c := n × (n+1) × (n+n−5)/6;
```

to make the inverse have the form described in the algorithm. The algorithm was translated to FORTRAN and tested with a matrix eigenvalue program on the CDC 1604 computer at UCSD.

The eigenvalues for the 20 × 20 test matrix are:

1.	1.000000
2.	1.000000
⋮	⋮
19.	.01636693
20.	−.02493833

REMARK ON ALGORITHM 52
A SET OF TEST MATRICES (John R. Herndon, *Comm. ACM*, Apr. 1961)

G. H. DUBAY
University of St. Thomas, Houston, Tex.

In the assignment statement

```
c := t×(t + 1)×(t + t − 5)/6;   (a)
```

the t is undefined. A suitable definition would be provided by preceding (a) with t := n;

REMARKS ON AND CERTIFICATION OF ALGORITHM 52
A SET OF TEST MATRICES [J. R. Herndon, *Comm. ACM*, Apr. 1961]

P. NAUR
Regnecentralen, Copenhagen, Denmark

In addition to inserting the correction indicated by H. E. Gilbert [*Comm. ACM* (Aug. 1961), 339] the algorithm was simplified by using the simultaneous assignment and by eliminating the local variables t and f. The resulting algorithm is as follows:

```
procedure TESTMATRIX(n,A);
value n; integer n; real array A;
comment ALG. 52: This procedure places in A an n × n matrix
  whose inverse and eigenvalues are known. The nth row and the
  nth column of the inverse are the set: 1, 2, 3, ..., n. The matrix
  formed by deleting the nth row and the nth column of the in-
  verse is the identity matrix of order n−1;
begin integer i,j; real c,d;
c := n × (n+1) × (n+n−5)/6;
d := 1/c;
A[n,n] := −d;
for i := 1 step 1 until n−1 do
  begin
  A[i,n] := A[n,i] := d × i;
  A[i,i] := d × (c−i↑2);
  for j := 1 step 1 until i−1 do A[i,j] := A[j,i] := −d × i × j
  end
end TESTMATRIX;
```

This version of the algorithm was successfully run in the GIER ALGOL system together with the inversion procedures INVERSION II and gjr (see Certification of Algorithm 120 below). From the figures produced by INVERSION II it looks as if the determinant of these matrices is given by $6/(n(n+1)(5-2n))$, which is also the value of the element $A[n,n]$. For $n > 3$ the absolutely greatest element is $A[1,1] = 1 + A[n,n]$.

CERTIFICATION OF ALGORITHM 52
A SET OF TEST MATRICES [J. R. Herndon, *Comm. ACM*, Apr. 1961]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The algorithm was corrected as recommended by H. E. Gilbert in his certification [*Comm. ACM*, Aug. 1961] and then successfully run using the Elliott ALGOL translator on the National-Elliott 803. The matrices so generated were used to test the matrix inversion procedure GJR given by H. R. Schwarz in his article "An Introduction to ALGOL" [Comm. ACM, Feb. 1962].

ADDITIONAL REMARKS ON ALGORITHM 52 A SET OF TEST MATRICES [J. R. Herndon, *Comm. ACM* (Apr. 1961), 180]

P. NAUR
Regnecentralen, Copenhagen, Denmark

From an inspection of the results of eigenvalue-finding algorithms I conclude that all but two of the eigenvalues of TESTMATRIX are unity while the two remaining are given by the expressions $6/(p\times(n+1))$ and $p/(n\times(5-2\times n))$ where

$$p = 3 + \text{sqrt}\ ((4\times n-3) \times (n-1) \times 3/(n+1)).$$

These expressions have been used for the determination of absolute errors of the eigenvalues calculated by JACOBI, Algorithm 85, and Householder Tridiagonalisation, etc. as reported below. They were also used to calculate the following table (using GIER ALGOL, with 29 significant bits):

n	*Determinant*	*Eigenvalues Differing from unity*	
3	−.500 000 00	.224 744 87	−2.224 744 9
4	−.100 000 00	.153 112 89	−.653 112 89
5	−.040 000 000	.113 238 08	−.353 238 08
6	−.020 408 163	.088 290 570	−.231 147 71
7	−.011 904 762	.071 428 571	−.166 666 67
8	−.007 575 757 6	.059 386 081	−.127 567 90
9	−.005 128 205 2	.050 422 549	−.101 704 60
10	−.003 636 363 6	.043 532 383	−.083 532 383
11	−.002 673 796 8	.038 097 478	−.070 183 039
12	−.002 024 291 5	.033 718 770	−.060 034 559
13	−.001 569 858 7	.030 128 103	−.052 106 125
14	−.001 242 236 0	.027 139 206	−.045 772 747
15	−.001 000 000 0	.024 619 013	−.040 619 013
16	−.000 816 993 47	.022 470 157	−.036 359 046
17	−.000 676 132 52	.020 619 902	−.032 790 288
18	−.000 565 930 96	.019 012 916	−.029 765 605
19	−.000 478 468 90	.017 606 429	−.027 175 807
20	−.000 408 163 27	.016 366 903	−.024 938 332

The figures for $n = 20$ agree very well with the results quoted by H. E. Gilbert in his certification [*Comm. ACM 4* (Aug. 1961), 339].

ALGORITHM 53
NTH ROOTS OF A COMPLEX NUMBER

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
procedure NTHROOT (n, r, u, REAL, UNREAL); value
          n, r, u; integer n;
          real r, u; real array REAL, UNREAL;
comment This procedure computes the n roots of the equation
  x^n = r+ui. The real parts of the roots are stored in the vector
  REAL [ ]. The imaginary parts are stored in the corresponding
  locations in the vector UNREAL [ ];
begin     integer n1, n2; real en, th, s, th 1;
          REAL [n] := 0;
          en := 1/n;
          if u=0 then
            begin s := (abs(r)) ↑ en;
            th := 0,
            go to main end;
          if r=0 then
            begin s := (abs(u)) ↑ en;
            th := 1.5707963;
            if u < 0 then
              th := −th
            go to main end;
            s := (r × r+u × u) ↑ (en/2);
            th := arctan (u/r);
main:       if r < 0 then
            th := th + 3.1415926;
          th := en × th;
          th1 := 6.2831853 × en;
          for n2 := 1 step 1 until n do
            begin REAL [n2] := s × cos (th);
            UNREAL [n2] := s × sin (th);
            th = th+th 1 end
end NTHROOT;
```

REMARK ON ALGORITHM 53
Nth ROOTS OF A COMPLEX NUMBER (John R. Herndon, *Comm. ACM 4*, Apr. 1961)

C. W. NESTOR, JR.
Oak Ridge National Laboratory, Oak Ridge, Tennessee

A considerable saving of machine time for $N \geqq 3$ would result from the use of the recursion formulas for the sine and cosine in place of an entry into a sine-cosine subroutine in the do loop associated with the Nth roots of a complex number. That is, one could use

$$\sin (n + 1)\theta = \sin n\theta \cos\theta + \cos n\theta \sin\theta$$
$$\cos (n + 1)\theta = \cos n\theta \cos\theta - \sin n\theta \sin\theta,$$

at the cost of some additional storage.

We have found this procedure to be very efficient in problems dealing with Fourier analysis, as suggested by G. Goerzel in chapter 24 of *Mathematical Methods for Digital Computers*.

ALGORITHM 54
GAMMA FUNCTION FOR RANGE 1 TO 2
JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
real procedure  Q(x);  value x;  real x,
comment  This procedure computes Γ(x) for 1 ≦ x ≦ 2. This is
  a reference procedure for the more general gamma function
  procedure. Γ(x) = Q(x−1);
begin           Q := (((((((0.035868343 × x − 0.19352782) × x
                  + 0.48219939) × x − 0.75670408) × x
                  + 0.91820686) × x − 0.89705694) × x
                  + 0.98820589) × x − 0.57719165) × x + 1.0
end             Q;
```

REMARKS ON:
ALGORITHM 34 [S14]
GAMMA FUNCTION
[M. F. Lipp, *Comm. ACM 4* (Feb. 1961), 106]
ALGORITHM 54 [S14]
GAMMA FUNCTION FOR RANGE 1 TO 2
[John R. Herndon, *Comm. ACM 4* (Apr. 1961), 180]
ALGORITHM 80 [S14]
RECIPROCAL GAMMA FUNCTION OF REAL ARGUMENT
[William Holsten, *Comm. ACM 5* (Mar. 1962), 166]
ALGORITHM 221 [S14]
GAMMA FUNCTION
[Walter Gautschi, *Comm. ACM 7* (Mar. 1964), 143]
ALGORITHM 291 [S14]
LOGARITHM OF GAMMA FUNCTION
[M. C. Pike and I. D. Hill, *Comm. ACM 9* (Sept. 1966), 684]

M. C. PIKE AND I. D. HILL (Recd. 12 Jan. 1966)
Medical Research Council's Statistical Research Unit,
University College Hospital Medical School,
London, England

Algorithms 34 and 54 both use the same Hastings approximation, accurate to about 7 decimal places. Of these two, Algorithm 54 is to be preferred on grounds of speed.

Algorithm 80 has the following errors:
(1) *RGAM* should be in the parameter list of *RGR*.
(2) The lines
if $x = 0$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x = 1$ **then begin** *RGR* := 1; **go to** *EXIT* **end**
should each be followed either by a semicolon or preferably by an **else**.
(3) The lines
if $x = 1$ **then begin** *RGR* := $1/y$; **go to** *EXIT* **end**
and
if $x < -1$ **then begin** $y := y \times x$; **go to** *CC* **end**
should each be followed by a semicolon.
(4) The lines
BB: **if** $x = -1$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x > -1$ **then begin** *RGR* := *RGAM*(x); **go to** *EXIT* **end**
should be separated either by **else** or by a semicolon and this second line needs terminating with a semicolon.
(5) The declarations of **integer** i and **real array** B[0:13] in *RGAM* are in the wrong place; they should come immediately after
begin real z;

With these modifications (and the replacement of the array B in *RGAM* by the obvious nested multiplication) Algorithm 80 ran successfully on the ICT Atlas computer with the ICT Atlas ALGOL compiler and gave answers correct to 10 significant digits.

Algorithms 80, 221 and 291 all work to an accuracy of about 10 decimal places and to evaluate the gamma function it is therefore on grounds of speed that a choice should be made between them. Algorithms 80 and 221 take virtually the same amount of computing time, being twice as fast as 291 at $x = 1$, but this advantage decreases steadily with increasing x so that at $x = 7$ the speeds are about equal and then from this point on 291 is faster—taking only about a third of the time at $x = 25$ and about a tenth of the time at $x = 78$. These timings include taking the exponential of *log-gamma*.

For many applications a ratio of gamma functions is required (e.g. binomial coefficients, incomplete beta function ratio) and the use of algorithm 291 allows such a ratio to be calculated for much larger arguments without overflow difficulties.

ALGORITHM 55
COMPLETE ELLIPTIC INTEGRAL OF THE FIRST KIND

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
real procedure  ELLIPTIC 1(k); value k; real k;
comment This procedure computes the elliptic integral of the
  first kind K(k, π/2);
begin           real t;
                t := 1−k × k;
                ELLIPTIC 1 := (((0.032024666 × t +
                    0.054555509) × t
                  + 0.097932891) × t + 1.3862944)
                  − (((0.010944912 × t + 0.060118519) × t
                  + 0.12475074) × t + 0.5) × log (t)
end             ELLIPTIC 1;
```

CERTIFICATION OF ALGORITHM 55
COMPLETE ELLIPTIC INTEGRAL OF THE FIRST KIND [John R. Herndon, *Comm. ACM*, Apr. 1961] and
CERTIFICATION OF ALGORITHM 149
COMPLETE ELLIPTIC INTEGRAL [J. N. Merner, *Comm. ACM*, Dec. 1962]

HENRY C. THACHER, JR.*
Reactor Eng. Div., Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

The bodies of Algorithm 55 and of the second procedure of Algorithm 149 were tested on the LGP-30 computer using SCALP, the Dartmouth "LOAD-AND-GO" translator for a substantial subset of ALGOL 60. The floating-point arithmetic for this translator carries 7+ significant digits.

In addition to modifications required because of the limitations of the SCALP subset, the following need correction:

In Algorithm 55:

1. The constant 0.054555509 should be 0.054544409.
2. The function *log* should be *ln*.

In procedure ELIP 2 of Algorithm 149, the statement $a := c$ should be $a := C$.

The parameters of Algorithm 149 are related to the complete elliptic integral of the first kind by: $K = a \times ELIP(a, b)$ where the parameter $m = k^2 = 1 - b/a$.

The maximum approximation error in Algorithm 55 is given by Hastings as about $0.6_{10}-6$. In addition there is the possibility of serious cancellation error in forming the complementary parameter $t = 1 - k \times k$. For k near 1, errors as great as 4 significant digits were sustained. In these regions, the complementary parameter itself is a far more satisfactory parameter.

The accuracy obtainable with Algorithm 149 is limited only by the arithmetic accuracy and the amount of effort which it is desired to expend. Six-figure accuracy was obtained with 5 applications of the arithmetic-geometric mean for $a = 1000$, $b = 2$, and with one application for $a = 500$, $b = 500$.

Neither algorithm is satisfactory for $k = 1$. The behavior for Algorithm 55 will be governed by the error exit from the logarithm procedure. Under these circumstances, Algorithm 149 goes into an endless loop. Algorithm 149 may also go into an endless loop of the terminating constant ($_{10}-8$ in the published algorithm) is too small for the arithmetic being used. For the SCALP arithmetic it was found necessary to increase this tolerance to $5.0_{10}-7$. The resulting values of the elliptic integrals were, however, accurate to within 2 in the 7th significant digit (6th decimal).

The relative efficiency of the two algorithms will depend strongly on the efficiency of the square-root and logarithm subroutines. With most systems, Algorithm 55 will provide sufficient accuracy, and will be more efficient. If a square-root operation or a highly efficient square-root subroutine is available, Algorithm 149 may well be the better method.

ALGORITHM 56
COMPLETE ELLIPTIC INTEGRAL OF THE SECOND KIND

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
real procedure ELLIPTIC 2(k); value k; real k:
comment This procedure computes the elliptic integral of the
  second kind E(k, π/2);
begin     real t;
          t := 1 − k × k;
          ELLIPTIC 2 := (((0.040905094 × t +
              0.085099193) × t
            + 0.44479204) × t + 1.0 − (((0.01382999 × t
            + 0.08150224) × t + 0.24969795) × t) × log (t)
end       ELLIPTIC 2;
```

CERTIFICATION OF ALGORITHM 56 [S21]
COMPLETE ELLIPTIC INTEGRAL OF THE SECOND KIND

[J. R. Herndon, *Comm. ACM 4*, (Apr. 1961), 180]

GERHARD MEIDELL LARSSEN (Recd. 9 Aug. 1965)
Institut für Statik und Dynamik der Luft- und Raumfahrtkonstruktionen mit Rechengruppe der Luftfahrt, Technische Hochschule, Stuttgart, Germany

Algorithm 56 was run on a UNIVAC 1107 using the UNIVAC 1107 ALGOL 60 compiler (dated January 25, 1965). The single-precision floating-point arithmetic of this translator carries eight significant digits.

Two syntactical errors were removed from the algorithm:

1. The line

ELLIPTIC 2 := (((0.040905094 × *t* +

was changed to

ELLIPTIC 2 := ((0.040905094 × *t* +

2. The function *log* was changed to *ln*.

In addition, the statement

t := 1−*k* × *k*

was removed from the algorithm and the complementary parameter itself used as input to the procedure:

real procedure *ELLIPTIC* 2 (*t*); **value** *t*; **real** *t*;

to avoid cancellation error for values of k near 1. [While the use of t as input parameter is good computationally, the name of the procedure is then slightly misleading.—J.G.H.]

Several values of the complete elliptic integral of the second kind were computed for $1 \geq t > 0$. The maximum error was found to be about $7_{10}-7$, compared with A. M. Legendre, Tafeln der Elliptischen Normalintegrale, Stuttgart, 1931. For $t = 0$ an error exit from the *ln* routine takes place.

ALGORITHM 57
BER OR BEI FUNCTION

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
real procedure BERBEI (r, z); value r, z; real r, z;
comment This procedure computes ber(z) if r is set equal to
  zero. bei(z) is produced if r equals 1.0;
begin
                real s, k, c, f, t;
                if r = 0 then
                  s := 1
                else
                  s := (z × z)/4;
                k := s;
                f := z × z;
                f := f × f;
                for c := 2 step 2 until 100 do
                  begin
                    if s = s + k then
                      go to gate;
                    t := (c+r) × (c+r−1);
                    k := −0.0625 × k × f/(t × t);
                    s := s+k end;
gate: BERBEI := s
end BERBEI;
```

CERTIFICATION OF ALGORITHM 57
BER OR BEI FUNCTION [J. R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

A. P. RELPH
The English Electric Co. Whetstone, England

Algorithm 57 was translated using the DEUCE ALGOL compiler. No corrections were required, and the results were satisfactory.

CERTIFICATION OF ALGORITHM 57
BER OR BEI FUNCTION [John R. Herndon, *Comm. ACM*, Apr. 1961]

HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of Algorithm 57 was tested on the LGP-30 using the ALGOL 60 translator developed by the Dartmouth College Computer Center. No syntactical errors were found. For $z = 0.1(0.1)1.0$, with a 7+ significant decimal arithmetic routine, the program gave results with errors less than 5 (and for $z = 1(1)5$ less than 12) in the seventh digit. For large values of z, serious cancellation errors may occur. For example, for $z = 20$, more than 2 decimals of significance can be lost in this way.

ALGORITHM 58
MATRIX INVERSION

DONALD COHEN
Burroughs Corporation, Pasadena, Calif.

```
procedure invert (n) array: (a);
comment  matrix inversion by Gauss-Jordan elimination;
    value n;
    array a;  integer n;
begin
    array b, c [1:n];  integer i, j, k, ℓ, p;
    integer array z [1:n];
        for j := 1 step 1 until n do z[j] := j;
        for i := 1 step 1 until n do begin
        k := i;  y := a[i, i];  ℓ := i − 1;  p := i + 1;
        for j := p step 1 until n do begin
        w := a[i, j];  if abs(w) > abs(y) then begin
        k := j;  y := w end end;
        for j := 1 step 1 until n do begin
        c[j] := a[j, k];  a[j, k] := a[j, i];
        a[j, i] := −c[j]/y;  b[j] := a[i, j] := a[i, j]/y end  ;
        a[i, i] := 1/y;  j := z[i];  z[i] := z[k];  z[k] := j  ;
        for k := 1 step 1 until ℓ, p step 1 until n do
        for j := 1 step 1 until ℓ, p step 1 until n do
        a[k, j] := a[k, i] − b[j] × c[k] end;  ℓ := 0  ;
back:   ℓ := ℓ + 1;  k := z[ℓ];  if ℓ ≦ n then begin
        for j := ℓ while k ≠ j do begin
        for i := 1 step 1 until n do begin
        w := a[j, i];  a[j, i] := a[k, i];  a[k, i] := w end  ;
        go to back end
        end invert.
```

CERTIFICATION OF ALGORITHM 58
MATRIX INVERSION (Donald Cohen, *Comm. ACM 4*, May 1961)

RICHARD A. CONGER
Yalem Computer Center, St. Louis University, St. Louis, Mo.

Invert was hand-coded in FORTRAN for the IBM 1620. The following corrections were found necessary:

The statement $a_{k,j} := a_{k,i} - b_j \times c_k$ *should be*

$$a_{k,j} := a_{k,j} - b_j \times c_k$$

The statement **go to** back *should be changed to*

$$i := z_k;\ z_k := z_j;\ z_j := i;\ \textbf{go to}\ \text{back}$$

After these corrections were made, the program was checked by inverting a 6×6 matrix and then inverting the result. The second result was equal to the original matrix within round-off.

CERTIFICATION OF ALGORITHM 58
MATRIX INVERSION [Donald Cohen, *Comm. ACM*, May, 1961]

RICHARD GEORGE*
Particle Accelerator Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

This procedure was programmed in FORTRAN and reduced to machine code mechanically. It was run on the Argonne-built computing machine, GEORGE. A floating-point routine was used which allows maximum accuracy to 31 bits.

There are a number of errors of various types:

(1) There are eight **begin**'s and only seven **end**'s.

(2) The line

$$a[k, j] := a[k, i] - b[j] \times c[k]\ \ \textbf{end};$$

should be

$$a[k, j] := a[k, j] - b[j] \times c[k]\ \ \textbf{end};$$

(3) The permutation of rows of the inverted matrix and permutation of elements of the integer array z must be carried out simultaneously. This algorithm fails to do this, and consequently the matrix at the time of exit from the procedure is left in a permuted condition.

(4) The algorithm permits the statement

$$k := z[l];$$

to be executed even though the declarations place an upper limit of n on the integer array z, and the test for $l \leqq n$ has not yet been made. Obviously, Mr. Cohen's compiling system would allow an out-of-bounds array look-up. One could easily incorporate into an ALGOL compiler a guard against such illicit array references, and therefore the published algorithm might be considered machine dependent.

(5) This algorithm requires $3n^2$ divisions, most of which are unnecessary. By inserting the statement

$$y := 1.0/y;$$

at the proper place, one may accomplish the obvious economy of reducing this to only n divisions plus $2n^2$ multiplications.

(6) If a matrix should be singular (or nearly so), some pivot element will be zero (or very small), and a test should be made, with provision for a jump to *ALARM*, a non-local label.

(7) The identifiers w and y should be declared within this procedure, to avoid trouble.

(8) This algorithm omits calculation of the determinant of the matrix. This could be computed with very little extra effort.

The revised algorithm was then tested on the LGP-30 computer, using ALGOL-30, a small subset of ALGOL. Within the restrictions of this subset, the program worked satisfactorily on test matrices.

REMARK ON ALGORITHM 58
MATRIX INVERSION [Donald Cohen, *Comm. ACM*, May, 1961]

GEORGE STRUBLE
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For the last seven lines, beginning with $a[k, j] := a[k, i]$, substitute:

```
a[k, j] := a[k, j] − b[j] × c[k] end;
l := 0;
back:  l := l+1;
again:  k := z[l];
if k ≠ l then
  begin for i := 1 step 1 until n do
    begin w := a[l, i];
          a[l, i] := a[k, i];
          a[k, i] := w end;
    z[l] := z[k];
    z[k] := k;
    go to again end;
  else if l ≠ n go to back
end invert
```

REMARK ON ALGORITHM 58
MATRIX INVERSION [D. Cohen, *Comm. ACM*, May 61]

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invert was run on FACIT EDB using FACIT-ALGOL 1. Some changes in the procedure had to be made:

1. y and w had to be declared in the procedure-body as **real** y, w;

2. The last part of the procedure starting with $l := 0$; which should interchange the matrix rows did not work correctly, even with the corrections proposed by R. A. Conger [*Comm. ACM*, June 62]. We propose the following code:

```
for l := 1 step 1 until n do begin
k := z[l];  for j := l while k ≠ j do begin
for i := 1 step 1 until n do begin
w := a[j, i];  a[j, i] := a[k, i];  a[k, i] := w end;
i := z[k];  z[k] := z[j];  k := z[j] := i end end end invert
```

If the matrix a is singular, the value of the pivot element y will once be zero or very nearly zero and division by zero would occur in the course of the calculation. It would therefore be advantageous to introduce an empirical tolerance parameter *epsilon* into the procedure.

To calculate the determinant of the matrix a it is only necessary to put three more statements into the code. With these augmentations *invert* should read:

```
procedure invert (n, a, epsilon, determinant);
value n, epsilon;  real epsilon, determinant;
array a;  integer n;
begin real y, w;  integer i, j, k, l, p;
array b, c[1:n];  integer array z[1:n];
determinant := 1;
```

followed by the same code as before until:

```
y := w end end;
determinant := y × determinant;
if k ≠ i then determinant := −determinant;
if abs (y) < epsilon then go to singular;
```

followed by the same code as before with the changes mentioned in the certification by R. A. Conger [*Comm. ACM*, June 62] and the changes given above. *singular* should be a nonlocal label in the main program.

ALGORITHM 59

ZEROS OF A REAL POLYNOMIAL BY RESULTANT PROCEDURE

E. H. BAREISS and M. A. FISHERKELLER

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```
procedure RES (n, c, alpha, mu, re, im, rt, gc) ; value n,
          c, alpha ; integer n, alpha ; integer array
          mu ; array c, re, im, rt, gc ;
comment   RES finds simultaneously all zeros of a polynomial of
    degree n with real coefficients, cj (j = 0, ... n), where cn
    is the constant term. The real part, rei , and imaginary part,
    imi , of each zero, with corresponding multiplicity, mui , and
    remainder term, rti , (i = 1, ... , n), are found and a poly-
    nomial with coefficients gcj (j = 0, ... , n), is generated from
    these zeros. Alpha provides an option for local or nonlocal
    selection of M, the number of root-squaring iterations, and
    delta and epsilon, acceptance criteria. If alpha = 1, these
    parameters are assigned locally. If alpha = 2, M, delta and
    epsilon are set equal to the global parameters Mp, deltap,
    and epsilonp, respectively. In cases where zeros may be found
    more than once, the superfluous ones are eliminated by fac-
    torization. The method has been described by E. H. Bareiss
    (J. ACM 7, Oct. 1960, pp. 346-386). ;
    begin integer M ; real delta, epsilon ; switch U :=
    U1, U2 ;
    go to U [alpha];
U1:           M := 10 ; delta := 0.2 ; epsilon := 10^-8 ;
              go to START ;
U2:           M := Mp ; delta := deltap ; epsilon :=
              epsilonp ;
START:        begin integer CT, nu, nuc, beta, m, j, jc, k,
              i, p ; Boolean ROOT ;
              real X, Y, GX, rp ; array a, ac [0:n, 0:M],
              R, Rc, t [0:n],
                  s [-1:n], ag [-2:n], rh, q, G, F [1:2×n] ;
              switch S := S1, S2 ; switch T := T1, T2 ;
              switch V := V1, V2 ;
              real procedure min (u,v) ; real u,v ;
                  min := if u ≦ v then u else v ;
              real procedure SYND (W, Q, I, T) ;
              integer I ; real W, Q ;
                  array T ;
SYNTHETIC     begin s [-1] := 0 ; s [0] := T [0] ; for
  DIV:        m := 1 step 1 until I do
                  s [m] := T [m] - W*s [m - 1] - Q×s
              [m - 2] ;
              if Q = 0 then SYND := abs (s[I]) else
                  SYND := abs (W/2×s [I - 1] + s[I])
              end SYND ;
              CT := beta := 1 ; for j := 0 step 1 until
              n do a [j,0] := c[j] ;
SQUARING      begin integer e1 ; real h ; for m :=
  OPERATION:  1 step 1 until M do
              begin for j := 1 step 1 until n do
              begin h := 0 ; for e1 := 1 step 1 until
              min (n - j, j) do
                  h := h + (-1) ↑ e1 × a [j - e1,m - 1] × a
              (j + e1 - 1] ;
                  a [j,m] := (-1) ↑ j × (a [j, m - 1] ↑
                  2 + 2×h) end end end ;
              for j := 0 step 1 until n do R [j] := (-1) ↑
              j×a [j, M - 1] ↑ 2/a [j,M] ;
                  j := 0 ; nu := 1 ;
RD:           if (1 - delta ≦ R [j]) ∧ (R [j] ≦ 1 + delta)
              then
              begin rp := (a [j,M]/a [j - nu, M]) ↑ (1/(2 ↑
              M×nu)) ;
              go to T [beta] end ;
1:            nu := nu + 1 ;
2:            j := j + 1 ; if j = n then go to S [beta]
              else go to RD ;
3:            nu := 1 ; go to 2 ;
T1:           rh [CT] := rp ; X := rp + epsilon × rp ;
              Y := X + epsilon × rp ;
              for k := 0 step 1 until n do t [k] := abs (c[k]) ;
                  F [CT] := SYND (Y,0,n,t) - SYND
                  (X,0,n,t) ;
                  G [CT] := SYND (rh [CT],0,n,c) ; if
                  F [CT] > G [CT] then
              begin ROOT := true ; q [CT] := 0 ;
              CT := CT + 1 ; F [CT] := F[CT - 1] end ;
              rh [CT] := -rp ; G [CT] := SYND (rh
              [CT],0,n,c) ;
              if F [CT] > G [CT] then begin ROOT :=
              true ; q [CT] := 0 ; CT := CT + 1 ;
              F [CT] := F [CT - 1] end ; if nu = 1 then
              go to 2 ;
              q [CT] := rp ↑ 2 ; nuc := nu ; jc := j ;
              for j := 0 step 1 until n do
              begin Rc [j] := R [j] ; ac [j,M] := a [j,M]
              end ;
RESULTANT:    begin real h ; array b [-1:n + 1,
              -1:n + 1], A [1:n],
                  r [0:n, 0:n], CB [-1:n + 1] ;
              b [-1,0] := CB [-1] := CB [n + 1] := 0 ;
              for j := 0 step 1 until n do
              CB [j] := c[j] ; b [0,0] := 1 ; for k :=
              1 step 1 until n do
              begin b [k,-1] := 0 ; for j := 0 step 1
              until k do
                  b [k + 1,j] := b [k,j - 1] - q [CT] × b
                  [k - 1,j] ;
                  b [k + 1, k + 1] := h := 0 ; for j :=
                  n - k step -1 until 0 do
                  h := h + (CB [j]×CB [k + j] - CB [j - 1]
                  ×CB[k + j + 1]) × q [CT] ↑ (n - k - j) ;
                  A [k] := (-1 ↑ k×h ; for j := 0 step
                  1 until k - 1 do
              begin r [0,j] := 0 ; r [k,j] := r [k - 1,j] +
              A [k] × b [k,j] end ,
                  r [k,k] := A[k] end ; beta := 2 ; for
                  j := 0 step 1 until n do
                  a [j,0] := r [n,j] end ; go to SQUAR-
                  ING OPERATION ;
T2:           if (rp/2) ↑ 2 ≧ q [CT] then go to 3 ; rh
              [CT] := rp ;
              G [CT] := SYND (rh [CT], q [CT], n,c) ;
```

```
                if F [CT] > G [CT] then
                begin CT := CT + 1 ; F [CT] := F
                [CT − 1] ; q [CT] := q [CT − 1] end ;
                rh [CT] := −rp ; G [CT] := SYND [rh [CT],
                q [CT], n,c) ;
                if F [CT] > G [CT] then begin CT := CT
                + 1 ; F [CT] := F [CT − 1] ;
                q [CT] := q [CT − 1] end ; go to 3 ;
S2:             for j := 0 step 1 until n do begin a [j,M] :=
                ac [j,M] ;
                R [j] := Rc [j] end ; j := jc ; beta := 1 ;
                if ROOT then go to 3 else
                    nu := nuc ; go to 1 ;
S1:             ag [−2] := ag [−1] := 0 ; ag [0] := 1 ;
                for j := 1 step 1 until n do
                ag [j] := 0 ; k := 1 ; i := n ; m := 1 ;
                for j := 0 step 1 until n do
                    t [j] := c [j] ;
MULT:           mu [m] := 0 ; p := if q [k] = 0 then 1
                else 2 ;
IT:             GX := SYND (rh [k], q [k],i,t) ; if F [k]
                > GX then
                begin for j := 1 step 1 until n do
                    ag [j] := ag [j] − rh [k] × ag [j − 1] + q
                    [k] × ag [j − 2] ;
                    mu [m] := mu [m] + p ; i := i − p ;
                    for j := 0 step 1 until i do
                    t [j] := s [j] ; go to IT end else if
                    mu [m] ≠ 0 then begin
                    rt [m] := G [k] ; go to V [p] end else
                    go to D ;
V1:             re [m] := rh [k] ; im [m] := 0 ; go to E ;
V2:             re [m] := rh [k]/2 ; im [m] := sqrt (q [k] −
                re [m] ↑ 2) ;
E:              m := m + 1 ;
D:              k := k + 1 ; if k ≦ CT ∧ m ≦ n then go to
                MULT ;
                for j := 0 step 1 until n do gc [j] := ag [j] end
                end RES
```

ALGORITHM 60
ROMBERG INTEGRATION

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```
real procedure rombergintegr (fct, ℓgr, rgr, ord) ;
  value ℓgr, rgr, ord ;
  real ℓgr, rgr; integer ord ; real procedure fct ;
  comment rombergintegr is the value of the integral of the
    function fct between the limits ℓgr and rgr, calculated by the
    algorithm of Romberg with an error term of the order
    2×ord+2, ord≧0 Computation time will roughly be doubled
    when ord is increased by 1;
  begin
    real array t[1 : ord+1];
    real ℓ, u, m ;
    integer f, h, j, n ;
    ℓ := rgr−ℓgr ;
    t[1] := (fct(ℓgr)+fct(rgr))/2 ;
    n := 1 ;
    for h := 1 step 1 until ord do
      begin u := 0 ;
        m := ℓ/(2×n) ;
        for j := 1 step 2 until 2×n−1 do
          u := u+fct(ℓgr+j×m) ;
        t[h+1] := (u/n+t[h])/2 ;
        f := 1 ;
        for j := h step −1 until 1 do
          begin f := 4×f ;
            t[j] := t[j+1]+(t[j+1]−t[j])/(f−1)
          end ;
        n := 2×n
      end ;
    rombergintegr := t[1]×ℓ
  end
```

CERTIFICATION OF ALGORITHM 60
ROMBERG INTEGRATION (F. L. Bauer, *Comm. ACM*, June, 1961)

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* Work supported by the U. S. Atomic Energy Commission.

This procedure was translated to the ACT III compiler language for the Royal Precision LGP-30 computer. This system provides 7+ significant decimal digits. The program was used to integrate x^n between the limits 0.01 and 1.1, and between the limits 1.1 and 0.01. The results in Table I were obtained. The pole at 0 for negative n affords a test of the reliability of the method when the higher derivatives of the integrand are large. The agreement between integrations in the forward and backward directions is an indication of the effects of round-off error.

It is apparent that the procedure gives results well within the noise level for the positive powers, and that even the effect of a closely adjacent singularity for the negative powers can be overcome.

The flexibility of the algorithm would be improved by adding to the formal parameters a procedure, check, to decide if sufficient accuracy had been obtained without carrying through the entire iteration. A possible form for this procedure would be:

TABLE I. INTEGRATION OF $\int_{0.01}^{1.1} x^n dx$ AND $\int_{1.1}^{0.01} x^n dx$

n	0	+12	+12	−1
True Value	1.0900000	.26555932	−.26555932	4.7004831
Order 1	1.0899997	.57076812	−.57076842	19.641113
Order 2	1.0899997	.30614608	−.30614626	10.656923
Order 5	1.0899991	.26555693	−.26555818	4.9017590
Order 10				4.7002345

n	−1	−5	−5
True Value	−4.7004831	$.25000000\times10^8$	-18.166667×10^8
Order 1	−19.641125	18.166655×10^8	$-.25000000\times10^8$
Order 2	−10.656929	8.4777719×10^8	-8.4777766×10^8
Order 5	−4.9017805	1.0408634×10^8	-1.0408640×10^8
Order 10	−4.7004402	$.25000715\times10^8$	$-.25000727\times10^8$
Order 12		$.24999291\times10^8$	$-.25001311\times10^8$

```
procedure check (t1, t2, f, exit);
  real t1, t2;
  label exit;
  integer f;
begin if abs ((t2 − t1) × f) / t1 < tolerance ∧ f > minimum order
  then go to exit end.
```

The global variables tolerance, which is the maximum relative difference between approximations of increasing order, and the minimum acceptable order should be selected by the programmer for the exigencies of the problem. A check of this sort is clearly not as sound as an a priori estimate of the necessary order, but is frequently an acceptable expedient.

The Romberg quadrature algorithm is analyzed in the following references:

Romberg, W. Vereinfachte numerische Integration. *Det Kongelinge Norske Videnskaber Selskab Forhandlinger 28*, (1955), 30-36.

Stiefel, E., and Rutishauser, H. Remarques concernant l'integration numerique. *Comptes Rendus Acad. Scil (Paris) 252*, (1961), 1899-1900.

CERTIFICATION OF ALGORITHM 60
ROMBERG INTEGRATION (F. L. Bauer, *Comm. ACM*, June 1961)

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Since August 1961, the Rombert Integration has been successfully applied in FORTRAN language to various problems on an IBM 1620. Due to its elegant method and the memory saving features, the Romberg Integration has succeeded other methods in our program library, e.g., the Newton-Cotes integration of order 10.

Reference is made to Stiefel, *Numerische Mathermatik* (Teubner Verlag. Stuttgart). Stiefel discusses in his book various methods of numerical integration including the Romberg algorithm.

CERTIFICATION OF ALGORITHM 60
ROMBERG INTEGRATION (F. L. Bauer, *Comm. ACM*, June 1961)

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REMARK ON ALGORITHM 60 [D1]
ROMBERG INTEGRATION [F. L. Bauer, *Comm. ACM 4* (June 1961) 255; *5* (Mar. 1962), 168; *5* (May 1962), 281]

HENRY C. THACHER, JR.* (Recd. 20 Feb. 1964 and 23 Mar. 1964)
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* Work supported by the U. S. Atomic Energy Commission.

The Romberg integration algorithm has been used with great success by many groups [1, 2], and appears to be among the most generally reliable quadrature methods available. It is, therefore, worth pointing out that it is not entirely foolproof, and that a significant class of integrands exists for which the extrapolated values are poorer estimates of the integral than the corresponding trapezoidal sums.

The validity of the Romberg procedure depends upon the possibility of expanding the error of the trapezoidal rule in powers of h^2, where h is the stepsize. One expansion of this type is the Euler-Maclaurin sum formula. An alternative expression may be obtained from the Fourier series expansion. The coefficients of h^{2r} in the Euler Maclaurin formula are proportional to the difference of the values of the $(2r+1)$-th derivative at the two ends of the range. Thus, any integral for which the odd derivatives of the integrand either vanish or are equal at the limits will not be improved by Romberg extrapolation. Among the common examples of such integrals are integrals of periodic functions over a period and integrals for which the derivatives vanish at both limits. An example of the last type is the integral approximation to the modified Hankel function [3], $e^x K_p(x) = \int_0^L e^{x(1-\cosh t)} \cosh(pt)dt$, where L is taken so large that the contribution of the integral from L to ∞ may be neglected. Several other examples are given under the heading "Exceptional cases" by Bauer, Rutishauser and Stiefele [7]. This paper is among the most extensive discussions of the Romberg method in English.

The algorithm also fails when the expansion of the error term contains other powers of h along with the even ones. Rutishauser [4] discusses estimating integrals of the form $\int_0^a f(x)\,dx = \int_0^a (\varphi(x)/\sqrt{x})\,dx$. If such integrals are estimated by the trapezoidal rule, assigning the value 0 to $f(0)$, the error may be expressed in the form $\sum c_k h^{2k} + \sqrt{h} \sum d_k h^k$. Although the standard Romberg extrapolation fails when applied to this sequence of estimates, Rutishauser presents a modified procedure which is effective.

The extrapolation is also invalid when the integrand is discontinuous, although this exception is trivial from the computational standpoint.

It has also been pointed out [5, 6] that the Romberg procedure may amplify round-off errors. The losses, while significant, do not appear prohibitive for most applications.

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ALGORITHM 61
PROCEDURES FOR RANGE ARITHMETIC

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```
begin
  procedure RANGESUM (a, b, c, d, e, f);
    real a, b, c, d, e, f;
  comment The term "range number" was used by P. S. Dwyer,
  Linear Computations (Wiley, 1951). Machine procedures for
  range arithmetic were developed about 1958 by Ramon Moore,
  "Automatic Error Analysis in Digital Computation," LMSD
  Report 48421, 28 Jan. 1959, Lockheed Missiles and Space Divi-
  sion, Palo Alto, California, 59 pp. If a ≦ x ≦ b and c ≦ y ≦ d,
  then RANGESUM yields an interval [e, f] such that e ≦ (x + y)
  ≦ f. Because of machine operation (truncation or rounding) the
  machine sums a + c and b + d may not provide safe end-points
  of the output interval. Thus RANGESUM requires a non-local
  real procedure ADJUSTSUM which will compensate for the
  machine arithmetic. The body of ADJUSTSUM will be de-
  pendent upon the type of machine for which it is written and so
  is not given here. (An example, however, appears below.) It
  is assumed that ADJUSTSUM has as parameters real v and w,
  and integer i, and is accompanied by a non-local real procedure
  CORRECTION which gives an upper bound to the magnitude
  of the error involved in the machine representation of a number.
  The output ADJUSTSUM provides the left end-point of the
  output interval of RANGESUM when ADJUSTSUM is called
  with i = −1, and the right end-point when called with i = 1.
  The procedures RANGESUB, RANGEMPY, and RANGEDVD
  provide for the remaining fundamental operations in range
  arithmetic. RANGESQR gives an interval within which the
  square of a range number must lie. RNGSUMC, RNGSUBC,
  RNGMPYC and RNGDVDC provide for range arithmetic with
  complex range arguments, i.e. the real and imaginary parts
  are range numbers;
  begin
    e := ADJUSTSUM (a, c, −1);
    f := ADJUSTSUM (b, d, 1)
  end RANGESUM;
  procedure RANGESUB (a, b, c, d, e, f);
    real a, b, c, d, e, f;
  comment RANGESUM is a non-local procedure;
  begin
    RANGESUM (a, b, −d, −c, e, f)
  end RANGESUB;
  procedure RANGEMPY (a, b, c, d, e, f);
    real a, b, c, d, e, f;
  comment ADJUSTPROD, which appears at the end of this
  procedure, is analogous to ADJUSTSUM above and is a non-
  local real procedure. MAX and MIN find the maximum and
  minimum of a set of real numbers and are non-local;
  begin
    real v, w;
    if a < 0 ∧ c ≧ 0 then
1:  begin
      v := c; c := a; a := v; w := d; d := b; b := w
    end 1;
    if a ≧ 0 then
2:  begin
      if c ≧ 0 then
3:  begin
        e := a × c; f := b × d; go to 8
      end 3;
      e := b × c;
      if d ≧ 0 then
4:    begin
        f := b × d; go to 8
      end 4;
      f := a × d; go to 8
5:  end 2;
    if b > 0 then
6:  begin
      if d > 0 then
      begin
        e := MIN(a × d, b × c);
        f := MAX(a × c, b × d); go to 8
      end 6;
      e := b × c; f := a × c; go to 8
    end 5;
    f := a × c;
    if d ≦ 0 then
7:  begin
      e := b × d; go to 8
    end 7;
    e := a × d;
8:  e := ADJUSTPROD (e, −1);
    f := ADJUSTPROD (f, 1)
  end RANGEMPY;
  procedure RANGEDVD (a, b, c, d, e, f);
    real a, b, c, d, e, f;
  comment If the range divisor includes zero the program
  exists to a non-local label "zerodvsr". RANGEDVD assumes a
  non-local real procedure ADJUSTQUOT which is analogous
  (possibly identical) to ADJUSTPROD;
  begin
    if c ≦ 0 ∧ d ≧ 0 then go to zerodvsr;
    if c < 0 then
1:  begin
      if b > 0 then
2:    begin
        e := b/d; go to 3
      end 2;
      e := b/c;
3:    if a ≧ 0 then
4:    begin
        f := a/c; go to 8
      end 4;
      f := a/d; go to 8
    end 1;
    if a < 0 then
5:  begin
      e := a/c; go to 6
    end 5;
    e := a/d;
6:  if b > 0 then
7:  begin
      f := b/c; go to 8
    end 7;
    f := b/d;
```

```
8:  e := ADJUSTQUOT (e, −1);  t := ADJUSTQUOT (f,1)
end RANGEDVD;
procedure RANGESQR (a, b, e, f);
  real a, b, e, f;
comment ADJUSTPROD is a non-local procedure;
begin
      if a < 0 then
1:    begin
        if b < 0 then
2:      begin
          e := b × b;   f := a × a;  go to 3
        end 2;
        e := 0;  m := MAX (-a,b);  f := m × m;  go to 3
      end 1;
      e := a × a;  f := b × b;
3:    ADJUSTPROD (e, −1);
      ADJUSTPROD (f, 1)
end  RANGESQR;
procedure  RNGSUMC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
  real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment  Rangesum is a non-local procedure;
begin
  RANGESUM (aL, aR, cL, cR, eL, eR);
  RANGESUM (bL, bU, dL, dU, fL, fU)
end  RNGSUMC;
procedure  RNGSUBC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
  real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment  RNGSUMC is a non-local procedure;
begin
  RNGSUMC (aL, aR, bL, bR, −cR, −cL, −dU, −dL, eL, eR,
  fL, fU)
end  RNGSUBC;
procedure  RNGMPYC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
  real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment  RANGEMPY, RANGESUB, and RANGESUM are
non-local procedures;
begin
  real L1, R1, L2, R2, L3, R3, L4, R4;
  RANGEMPY (aL, aR, cL, cR, L1, R1);
  RANGEMPY (bL, bU, dL, dU, L2, R2);
  RANGESUB (L1, R1, L2, R2, eL, eR);
  RANGEMPY (aL, aR, dL, dU, L3, R3);
  RANGEMPY (bL, bU, cL, cR, L4, R4);
  RANGESUM (L3, R3, L4, R4, fL, fU);
end  RNGMPYC;
procedure  RNGDVDC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
  real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment  RNGMPYC, RANGESQR, RANGESUM, and
RANGEDVD are non-local procedures;
begin
  real L1, R1, L2, R2, L3, R3, L4, R4, L5, R5;
  RNGMPYC (aL, aR, bL, bU, cL, cR, −dU, −dL, L1, R1, L2,
  R2);
  RANGESQR (cL, cR, L3, R3);
  RANGESQR (dL, dU, L4, R4);
  RANGESUM (L3, R3, L4, R4, L5, R5);
  RANGEDVD (L1, R1, L5, R5, eL, eR);
  RANGEDVD (L2, R2, L5, R5, fL, fU)
end  RNGDVDC
end
```

EXAMPLE

```
real procedure  CORRECTION (p);  real p;
comment  CORRECTION and the procedures below are in-
tended for use with single-precision normalized floating-point
arithmetic for machines in which the mantissa of a floating-point
number is expressible to s significant figures, base b. Limitations
of the machine or requirements of the user will limit the range of
p to b^m ≦ | p | < b^(n+1) for some integers m and n. Appropriate
integers must replace s, b, m and n below. Signal is a non-local
label. The procedures of the example would be included in the
same block as the range procedures above;
begin
    integer w;
    for w := m step 1 until n do
1:  begin
      if (b ↑ w ≦ abs (p)) ∧ (abs (p) < b ↑ (w + 1)) then
2:    begin
        CORRECTION := b ↑ (w+1−s);  go to exit
      end 2
    end 1;
    go to signal;
exit: end  CORRECTION;
real procedure  ADJUSTSUM (w, v, i);  integer i;
  real w, v;
comment  ADJUSTSUM exemplifies a possible procedure for use
with machines which, when operating in floating point addition,
simply shift out any lower order digits that may not be used. No
attempt is made here to examine the possibility that every digit
that is dropped is zero. CORRECTION is a non-local real pro-
cedure which gives an upper bound to the magnitude of the error
involved in the machine representation of a number;
begin
  real r, cw, cv, cr;
  r := w + v;
  if w = 0 ∨ v = 0 then go to 1;
  cw := CORRECTION (w);
  cv := CORRECTION (v);
  cr := CORRECTION (r);
  if cw = cv ∧ cr ≦ cw then go to 1;
  if sign (i × sign (w) × sign (v) × sign (r)) = −1 then go to 1;
  ADJUSTSUM := r + i × MAX (cw, cv, cr);  go to exit;
1: ADJUSTSUM := r;
exit: end  ADJUSTSUM;
real procedure  ADJUSTPROD (p, i);  real p;  integer i;
comment  ADJUSTPROD is for machines which truncate when
lower order digits are dropped. CORRECTION is a non-local real
procedure;
begin
    if p × i ≦ 0 then
1:  begin
      ADJUSTPROD := p;  go to out
    end 1;
    ADJUSTPROD := p + i × CORRECTION (p);
out:  end  ADJUSTPROD;
comment  Although ordinarily rounded arithmetic is preferable
to truncated (chopped) arithmetic, for these range procedures
truncated arithmetic leads to closer bounds than rounding does.
```

---

* These procedures were written and tested in the Burroughs 220 version of the ALGOL language in the summer of 1960 at Stanford University. The typing and editorial work were done under Office of Naval Research Contract Nonr-225(37). The author wishes to thank Professor George E. Forsythe for encouraging this work and for assistance with the syntax of ALGOL 60.

ALGORITHM 62
A SET OF ASSOCIATE LEGENDRE POLYNOMIALS OF THE SECOND KIND*

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

```
comment This procedure places a set of values of Q_n^m(x) in the
array Q[ ] for values of n from 0 to nmax for a particular value
of m and a value of x which is real if ri is 0 and is purely imaginary,
ix, ortherwise. R[ ] will contain the set of ratios of successive
values of Q. These ratios may be especially valuable when the
Q_n^m(x) of the smallest size is so small as to underflow the machine
representation (e.g. 10^-60 if 10^-51 were the smallest representable
number). 9.9 × 10^45 is used to represent infinity. Imaginary
values of x may not be negative and real values of x may not be
smaller than 1.

Values of Q_n^m(x) may be calculated easily by hypergeometric
series if x is not too small nor (n − m) too large. Q_n^m(x) can be
computed from an appropriate set of values of P_n^m(x) if x is near
1.0 or ix is near 0. Loss of significant digits occurs for x as small as
1.1 if n is larger than 10. Loss of significant digits is a major diffi-
culty in using finite polynomial representations also if n is larger
than m. However, QLEG has been tested in regions of x and n
both large and small;
procedure QLEG(m, nmax, x, ri, R, Q); value m, nmax, x, ri;
          real m, nmax, x, ri; real array R, Q;
begin real t, i, n, q0, s;
      n := 20;
      if nmax > 13 then
         n := nmax + 7;
      if ri = 0 then
         begin if m = 0 then
                       Q[0] := 0.5 × log((x + 1)/(x − 1))
                       else
               begin t := −1.0/sqrt(x × x − 1);
                       q0 := 0;
                       Q[0] := t;
                       for i := 1 step 1 until m do
                         begin s := (x+x)×(i−1)×t
                         ×Q[0]+(3i−i×i−2)×q0;
                         q0 := Q[0];
                         Q[0] := s end end;
         if      x = 1 then
                 Q[0] := 9.9 ↑ 45;
         R[n + 1] := x − sqrt(x × x − 1);
         for     i := n step −1 until 1 do
                 R[i] := (i + m)/((i + i + 1) × x
                 +(m − i − 1) × R[i + 1]);
         go to the end;
      if m = 0 then
         begin if x < 0.5 then
                 Q[0] := arctan(x) − 1.5707963 else
                 Q[0] := − arctan(1/x)end else
         begin t := 1/sqrt(x × x + 1);
         q0 := 0;
         Q[0] := t;
         for     i := 2 step 1 until m do
                 begin s := (x + x) × (i − 1) × t × Q[0]
                 +(3i + i × i − 2) × q0;
                 q0 := Q[0];
                 Q[0] := s end end;
      R[n + 1] := x − sqrt(x × x + 1);
         for  i := n step − 1 until 1 do
              R[i] := (i + m)/((i − m + 1) × R[i + 1]
              −(i + i + 1) × x);
         for  i := 1 step 2 until nmax do
              R[i] := − R[i];
the:  for i := 1 step 1 until nmax do
              Q[i] := Q[i − 1] × R[i]
end QLEG;
```

* This procedure was developed in part under the sponsorship of the Air Force Cambridge Research Center.

REMARK ON ALGORITHM 62
A SET OF ASSOCIATE LEGENDRE POLYNOMIALS OF THE SECOND KIND (John R. Herndon, *Comm. ACM 4* (July, 1961))

JOHN R. HERNDON
Stanford Research Institute, Menlo Park, California

In regard to Algorithm 62 in *Communications of the ACM*, two errors were found:

The 14th line of the procedure

```
for i := 1 step 1 until m do
```

should read

```
for i := 2 step 1 until m do
```

The 35th line

```
+(3i − iXi − 2)Xq0
```

should read

```
+(3i − i × i − 2) × q0
```

The procedure *QLEC* was developed from the standard recurrence formula

$$(n + m - 1)Q_{n-2}^m = (2n - 1)\cdot x\cdot Q_{n-1}^m - (n - m)Q_n^m.$$

Invert and multiply by $(n + m - 1)Q_{n-1}^m$.

$$\frac{Q_{n-1}^m}{Q_{n-2}^m} = \frac{(n + m - 1)}{(2n - 1)\cdot x - (n - m)Q_n^m/Q_{n-1}^m},$$

or

$$R_{n-1}^m = \frac{(n + m - 1)}{(2n - 1)\cdot x - (n - m)R_n^m}.$$

Analysis (and testing) shows that, for n large, this infinite continued fraction need only be carried to about eight terms for eight-digit accuracy if the final term is evaluated with the asymptotic value derived by setting

$$R_{n-1}^m = R_n^m, \quad \lim_{n\to\infty} R_n^m = x \pm \sqrt{x^2 - 1},$$

the minus sign being chosen since in general $Q_n^m < Q_{n-1}^m$. The formulas pertaining to purely imaginary parameters follow readily. The value of

$$Q_0^0(x) = \frac{1}{2}\log_e\frac{x + 1}{x - 1},$$

while

$$Q_1^0(x) = x \cdot Q_0^0(x) - 1,$$

and

$$Q_0^1(x) = \frac{-1}{\sqrt{x^2 - 1}}.$$

Other values are derived using the ratios $R_n^m(x)$ and/or the recurrence formula

$$Q_n^m = -\frac{2(m-1)x}{\sqrt{x^2-1}} Q_n^{m-1} + (n - m + 2)(n + m - 2)Q_n^{m-2}.$$

The derivation of the expression for $Q_0^0(ix)$ is not trivial and proceeds as follows:

$$i \cdot Q_0^0(ix) = \frac{1}{2}\log_e \frac{ix+1}{ix-1} = \frac{1}{2}\log_e \left[-\frac{x^2-1}{x^2+1} + \frac{2x}{x^2+1} \right]$$

$$e^{a+ib} = e^a \cdot e^{ib} = e^a \cos b + i \sin b.$$

Thus

$$\tan b = \frac{-2x}{1-x^2}$$

and

$$Q_0^0(ix) = (\arctan x - \pi/2)i.$$

ALGORITHM 63
PARTITION

C. A. R. HOARE
Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

```
procedure  partition (A,M,N,I,J);  value M,N;
           array A;  integer M,N,I,J;
comment  I and J are output variables, and A is the array (with
subscript bounds M:N) which is operated upon by this procedure.
Partition takes the value X of a random element of the array A,
and rearranges the values of the elements of the array in such a
way that there exist integers I and J with the following properties:
                M ≦ J < I ≦ N provided M < N
                A[R] ≦ X for M ≦ R ≦ J
                A[R] = X for J < R < I
                A[R] ≧ X for I ≦ R ≦ N
The procedure uses an integer procedure random (M,N) which
chooses equiprobably a random integer F between M and N, and
also a procedure exchange, which exchanges the values of its two
parameters;
begin   real X;  integer F;
        F := random (M,N);  X := A[F];
        I := M;  J := N;
up:     for I := I step 1 until N do
                  if X < A [I] then go to down;
        I := N;
down:   for J := J  step −1 until M do
                  if A[J]<X then go to change;
        J := M;
change: if I < J then begin exchange (A[I], A[J]);
                             I := I + 1; J := J − 1;
                             go to up
                       end
else    if I < F then begin exchange (A[I], A[F]);
                             I := I + 1
                       end
else    if F < J then  begin exchange (A[F], A[J]);
                             J := J − 1
                       end;
end     partition
```

CERTIFICATION OF ALGORITHMS 63, 64, 65
PARTITION, QUICKSORT, FIND [C. A. R. Hoare, *Comm. ACM*, July 1961]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The body of the procedure find was corrected to read:

```
begin integer I, J;
if M < N then begin partition (A, M, N, I, J);
                if K ≦ I then find (A, M, J, K)
                else if J ≦ K then find (A, I, N, K)
                end
end find
```

and the trio of procedures was then successfully run using the Elliott ALGOL translator on the National-Elliott 803.

The author's estimate of $\frac{1}{3}(N-M)1n(N-M)$ for the number of exchanges required to sort a random set was found to be correct. However, the number of comparisons was generally less than $2(N-M)1n(N-M)$ even without the modification mentioned below.

The efficiency of the procedure quicksort was increased by changing its body to read:

```
begin integer I, J;
if M < N−1 then begin partition (A, M, N, I, J);
                  quicksort (A, M, J);
                  quicksort (A, I, N)
                  end
else if N−M = 1 then begin if A[N] < A[M] then
                               exchange (A[M], A[N])
                     end
end quicksort
```

This alteration reduced the number of comparisons involved in sorting a set of random numbers by 4–5 percent, and the number of entries to the procedure partition by 25–30 percent.

CERTIFICATION OF ALGORITHMS 63, 64 AND 65, PARTITION, QUICKSORT, AND FIND, [*Comm. ACM*, July 1961]

B. RANDELL AND L. J. RUSSELL
The English Electric Company Ltd., Whetstone, England

Algorithms 63, 64, and 65 have been tested using the Pegasus ALGOL 60 Compiler developed at the De Havilland Aircraft Company Ltd., Hatfield, England.

No changes were necessary to Algorithms 63 and 64 (Partition and Quicksort) which worked satisfactorily. However, the comment that Quicksort will sort an array without the need for any extra storage space is incorrect, as space is needed for the organization of the sequence of recursive procedure activations, or, if implemented without using recursive procedures, for storing information which records the progress of the partitioning and sorting.

A misprint ('if' for 'if' on the line starting **'else if** $J \leqq K$ **then** ⋯') was corrected in Algorithm 65 (Find), but it was found that in certain cases the sequence of recursive activations of *Find* would not terminate successfully. Since *Partition* produces as output two integers J and I such that elements of the array $A[M:N]$ which lie between $A[J]$ and $A[I]$ are in the positions that they will occupy when the sorting of the array is completed, *Find* should cease to make further recursive activations of itself if K fulfills the condition $J < K < I$.

Therefore the conditional statement in the body of *Find* was changed to read

```
if K ≦ J then find (A,M,J,K)
else if I ≦ K then find (A,I,N,K)
```

With this change the procedure worked satisfactorily.

ALGORITHM 64
QUICKSORT

C. A. R. HOARE
Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

```
procedure  quicksort (A,M,N); value M,N;
             array A; integer M,N;
comment Quicksort is a very fast and convenient method of
sorting an array in the random-access store of a computer. The
entire contents of the store may be sorted, since no extra space is
required. The average number of comparisons made is 2(M−N) ln
(N−M), and the average number of exchanges is one sixth this
amount. Suitable refinements of this method will be desirable for
its implementation on any actual computer;
begin      integer I,J;
           if M < N then begin partition (A,M,N,I,J);
                               quicksort (A,M,J);
                               quicksort (A, I, N)
                         end
end        quicksort
```

CERTIFICATION OF ALGORITHMS 63, 64, 65 PARTITION, QUICKSORT, FIND [C. A. R. Hoare, *Comm. ACM*, July 1961]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The body of the procedure find was corrected to read:

```
begin integer I, J;
if M < N then begin partition (A, M, N, I, J);
                if K ≦ I then find (A, M, J, K)
                else if J ≦ K then find (A, I, N, K)
                end
end find
```

and the trio of procedures was then successfully run using the Elliott ALGOL translator on the National-Elliott 803.

The author's estimate of $\frac{1}{3}(N-M)1n(N-M)$ for the number of exchanges required to sort a random set was found to be correct. However, the number of comparisons was generally less than $2(N-M)1n(N-M)$ even without the modification mentioned below.

The efficiency of the procedure quicksort was increased by changing its body to read:

```
begin integer I, J;
if M < N−1 then begin partition (A, M, N, I, J);
                      quicksort (A, M, J);
                      quicksort (A, I, N)
                      end
else if N−M = 1 then begin if A[N] < A[M] then
                                 exchange (A[M], A[N])
                           end
end quicksort
```

This alteration reduced the number of comparisons involved in sorting a set of random numbers by 4–5 percent, and the number of entries to the procedure partition by 25–30 percent.

CERTIFICATION OF ALGORITHMS 63, 64 AND 65, PARTITION, QUICKSORT, AND FIND, [*Comm. ACM*, July 1961]

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Algorithms 63, 64, and 65 have been tested using the Pegasus ALGOL 60 Compiler developed at the De Havilland Aircraft Company Ltd., Hatfield, England.

No changes were necessary to Algorithms 63 and 64 (Partition and Quicksort) which worked satisfactorily. However, the comment that Quicksort will sort an array without the need for any extra storage space is incorrect, as space is needed for the organization of the sequence of recursive procedure activations, or, if implemented without using recursive procedures, for storing information which records the progress of the partitioning and sorting.

A misprint ('if' for '**if**' on the line starting '**else** if $J \leqq K$ **then** ...') was corrected in Algorithm 65 (Find), but it was found that in certain cases the sequence of recursive activations of *Find* would not terminate successfully. Since *Partition* produces as output two integers J and I such that elements of the array $A[M:N]$ which lie between $A[J]$ and $A[I]$ are in the positions that they will occupy when the sorting of the array is completed, *Find* should cease to make further recursive activations of itself if K fulfills the condition $J < K < I$.

Therefore the conditional statement in the body of *Find* was changed to read

```
if K ≦ J then find (A,M,J,K)
else if I ≦ K then find (A,I,N,K)
```

With this change the procedure worked satisfactorily.

ALGORITHM 65
FIND

C. A. R. HOARE
Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

```
procedure  find (A,M,N,K);  value M,N,K;
             array A;  integer M,N,K;
comment  Find will assign to A [K] the value which it would
have if the array A [M:N] had been sorted. The array A will be
partly sorted, and subsequent entries will be faster than the first;
begin      integer I,J;
           if M < N then begin partition (A, M, N, I, J);
                         if K≦I then find (A,M,I,K)
                         else if J≦K then find (A,J,N,K)
                         end
end        find
```

CERTIFICATION OF ALGORITHMS 63, 64, 65 PARTITION, QUICKSORT, FIND [C. A. R. Hoare, *Comm. ACM*, July 1961]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The body of the procedure find was corrected to read:

```
begin integer I, J;
if M < N then begin partition (A, M, N, I, J);
                if K ≦ I then find (A, M, J, K)
                else if J ≦ K then find (A, I, N, K)
                end
end find
```

and the trio of procedures was then successfully run using the Elliott ALGOL translator on the National-Elliott 803.

The author's estimate of $\frac{1}{3}(N-M)1n(N-M)$ for the number of exchanges required to sort a random set was found to be correct. However, the number of comparisons was generally less than $2(N-M)1n(N-M)$ even without the modification mentioned below.

The efficiency of the procedure quicksort was increased by changing its body to read:

```
begin integer I, J;
if M < N-1 then begin partition (A, M, N, I, J);
                      quicksort (A, M, J);
                      quicksort (A, I, N)
                      end
else if N-M = 1 then begin if A[N] < A[M] then
                                 exchange (A[M], A[N])
                           end
end quicksort
```

This alteration reduced the number of comparisons involved in sorting a set of random numbers by 4–5 percent, and the number of entries to the procedure partition by 25–30 percent.

CERTIFICATION OF ALGORITHMS 63, 64 AND 65, PARTITION, QUICKSORT, AND FIND, [*Comm. ACM*, July 1961]

B. RANDELL AND L. J. RUSSELL
The English Electric Company Ltd., Whetstone, England

Algorithms 63, 64, and 65 have been tested using the Pegasus ALGOL 60 Compiler developed at the De Havilland Aircraft Company Ltd., Hatfield, England.

No changes were necessary to Algorithms 63 and 64 (Partition and Quicksort) which worked satisfactorily. However, the comment that Quicksort will sort an array without the need for any extra storage space is incorrect, as space is needed for the organization of the sequence of recursive procedure activations, or, if implemented without using recursive procedures, for storing information which records the progress of the partitioning and sorting.

A misprint ('if' for '**if**' on the line starting '**else if** $J \leqq K$ **then** $\cdots$') was corrected in Algorithm 65 (Find), but it was found that in certain cases the sequence of recursive activations of *Find* would not terminate successfully. Since *Partition* produces as output two integers J and I such that elements of the array $A[M:N]$ which lie between $A[J]$ and $A[I]$ are in the positions that they will occupy when the sorting of the array is completed, *Find* should cease to make further recursive activations of itself if K fulfills the condition $J < K < I$.

Therefore the conditional statement in the body of *Find* was changed to read

```
if K ≦ J then find (A,M,J,K)
else if I ≦ K then find (A,I,N,K)
```

With this change the procedure worked satisfactorily.

ALGORITHM 66
INVRS

JOHN CAFFREY
Director of Research, Palo Alto Unified School District, Palo Alto, California

```
procedure Invrs (t) size : (n); value n; real array t; integer n;
comment Inverts a positive definite symmetric matrix t, of order n, by a simplified variant of the square root method. Replaces the n(n+1)/2 diagonal and superdiagonal elements of t with elements of t^-1, leaving subdiagonal elements unchanged. Advantages: only n temporary storage registers are required, no identity matrix is used, no square roots are computed, only n divisions are performed, and, as n becomes large, the number of multiplications approaches n^3/2;
begin integer i, j, s; real array v[1:n-1]; real y, pivot;
for s := 0 step 1 until n-1 do
begin pivot := 1.0/t[1,1];
    begin pivot := 1.0/t[1,1];
                comment If t[1,1] ≦ 0, t is not positive definite;
        for i := 2 step 1 until n do v[i-1] := t[1, i];
        for i := 1 step 1 until n-1 do
            begin t[i,n] := y := -v[i] × pivot;
            for j := i step 1 until n-1 do
            t[i, j] := t[i + 1, j +1] + v[j] × y
            end;
        t[n,n] := -pivot
    end;
            comment At this point, elements of t^-1 occupy the original array space but with signs reversed, and the following statements effect a simple reflection;
    for i := 1 step 1 until n do
    for j := i step 1 until n do t[i,j] := -t[i,j]
end Invrs
```

CERTIFICATION OF ALGORITHM 66
INVRS (J. Caffrey, Comm. ACM, July 1961)

B. RANDELL, C. G. BROYDEN.
Atomic Power Division, The English Electric Company, Whetstone, England.

INVRS was translated using the DEUCE ALGOL Compiler, and needed the following correction.

The repeat of the line,

```
begin pivot := 1.0/t[1, 1];
```

was deleted.

The compiled program, which used a 20 bit mantissa floating point notation, was tested using Wilson's matrix

5	7	6	5
7	10	8	7
6	8	10	9
5	7	9	10

and gave results

67.9982	−40.9991	−16.9995	9.9997
−40.9991	24.9995	9.9997	−5.9998
−16.9995	9.9997	4.9998	−2.9999
9.9997	−5.9998	−2.9999	1.9999

(The output routine completed the symmetric matrix)

INVRS will in fact invert non-positive symmetric matrices, the only restriction appearing to be that the leading minors of the matrix must be non-zero. The variable T[1, 1] takes as its successive values ratios of the (r + 1)th to the r th leadng minors of the matrix, and if it becomes zero the variable 'pivot' cannot be computed.

The following matrix, for which the successive values of T[1, 1] were +2, −2, −1, −0.6, +5 gave results correct to one unit in the fifth significant figure.

2	−3	1	−1	4
−3	2	−4	3	−2
1	−4	−3	2	4
−1	3	2	−2	−3
4	−2	4	−3	2

CERTIFICATION OF ALGORITHM 66
INVRS (J. Caffrey, *Comm. ACM*, July 1961)

JOHN CAFFREY
Palo Alto Unified School District, Palo Alto, California

INVRS was translated using the Burroughs 220 Algebraic Computer (BALCOM) at Stanford University, using 8-digit floating-point arithmetic. The misprint noted by Randell and Broyden (*Comm. ACM*, Jan. 1962, p. 50) was corrected, and the same example (Wilson's 4 × 4 matrix) was used as a test case. The resulting inverse was:

68.0000	−41.0000	−17.0000	10.0000
	25.0000	10.0000	−6.0000
		5.0000	−3.0000
			2.0000

It may also be useful to note that the determinant of the matrix may be obtained as the successive product of the pivots. That is, if t_i ($= T(1, 1)$) is the ith pivot of a matrix of order n,

$$\text{determinant} = \prod_i^n t_i .$$

For the above *input* example,

determinant = 1.0

Randell and Broyden's observation concerning the *apparent* limitation of INVRS to positive definite cases is correct: That is, any nonsingular real symmetric matrix (positive, indefinite, or negative) may be inverted using this algorithm. The original INVRS should therefore be modified as follows:

```
if pivot = 0 then go to singular;
```

Randell and Broyden's second example (of order 5) was also used as a test case, with the resulting inverse:

−.0000	.9999	.0000	.0000	.9999
	1.5333	−.7333	−.1333	.7999
		−.8666	−1.0666	−.5999
			−1.4666	−.1999
				.2000

determinant = −14.999999

An attempt to invert the *inverse* of the 4 × 4 segment of the Hilbert matrix, as presented by Randell (*Comm. ACM*, Jan. 1962, p. 50), yielded the following results:

.9999	.4999	.3333	.2499
	.3333	.2499	.1999
		.1999	.1666
			.1428

determinant = 6048020.6

ALGORITHM 67
CRAM

JOHN CAFFREY
Director of Research, Palo Alto Unified School District, Palo Alto, California

```
procedure CRAM (n, r, a) Result: (f); value n, r; integer
  n, r; real array a, f;
comment CRAM stores, via an unspecified input procedure
READ, the diagonal and superdiagonal elements of a square sym-
metric matrix e, of order n, as a pseudo-array of dimension
1:n(n + 1)/2. READ (u) puts one number into u. Elements e[i, j]
are addressable as a[c + j], where c = (2n − i)(i − 1)/2 and c[i + 1]
may be found as c[i] + n − i. Since c[1] = 0, it is simpler to develop
a table of the c[i] by recursion, as shown in the sequence labelled
"table". Further manipulation of the elements so stored is illus-
trated by premultiplying a rectangular matrix f, of order n, r, by
the matrix e, replacing the elements of f with the new values, re-
quiring a temporary storage array v of dimension 1:n;
begin integer i, j, k, m; real array v[1:n]; real s;
  integer array c[1:n];
table: j := − n; k := n + 1; for i := 1 step 1 until n do
       begin
       j := j + k − i; c[i] := j end;
load: for i := 1 step 1 until n do
      begin for j := i step 1 until n do READ (v[j]); m :=
      c[i];
      for k := i step 1 until n do a[m + k] := v[k] end;
premult: for j := 1 step 1 until r do
         begin for i := 1 step 1 until n do
               begin s := 0.0;
                 for k := 1 step 1 until i do
                 begin m := c[k]; s := s + a[m + i]
                   ×f[k, j] end;
                 for k := i + 1 step 1 until n do
                     s := s + a[m + k] × f[k, j]; v[i] = s
               end;
               for k := 1 step 1 until n do f[k, j] = v[k]
         end
end CRAM
```

CERTIFICATION OF ALGORITHM 67
CRAM (J. Caffrey, *Comm. ACM 4* (July 1961), 322)

A. P. RELPH
Atomic Power Div., The English Electric Co., Whetstone, England

CRAM was translated using the DEUCE ALGOL compiler with the following corrections:

V[i] = S *was changed to* V[i] := S
f[k,j] = V[k] *was changed to* f[k,j] := V[k]

It is quicker not to use the table of the C[i] in the "load" sequence and instead use the following sequence:

```
load: m := n × (n+1)/2;
      for i := 1 step 1 until m do READ (a[i]);
```

ALGORITHM 68
AUGMENTATION
H. G. RICE
Computer Sciences Corp., Palos Verdes, Calif.

```
real procedure Aug(x,y); value x,y; integer x,y;
comment This algorithm makes use of the implicitly defined recursive properties of ALGOL procedures to compute the augment of x by y, using the basic technique of incrementation by unit step size;
begin Aug := if x = 0 then (if y > x then (Aug(y − 1, x) + 1)
  else y)
else Aug(x − 1, y + 1) end Aug
```

CERTIFICATION OF ALGORITHM 68
AUGMENTATION (H. G. Rice, *Comm. ACM*, Aug. 1961)
L. M. BREED
Stanford University, Stanford, Calif.

AUGMENTATION was transliterated into BALGOL for the Burroughs 220, and proved successful in a number of test cases. However, the following algorithm has exactly the same effect and is considerably simpler:

```
real procedure Aug(x, y); value x, y; integer x, y;
begin if x<0 then L : go to L else Aug := x+y end Aug
```

ALGORITHM 69
CHAIN TRACING
BRIAN H. MAYOH
Regnecentralen, Gl. Carlsbergvet. 2, Copenhagen.

```
procedure CHAIN tracing (iteration counter, number of
        identifiers, number of identifier links, final linkage
        matrix, couples);
    Boolean array final linkage matrix;
    integer array couples;
    integer iteration counter, number of identifiers, number of
      identifier links;
begin comment This procedure is given a list of pairs of inte-
    gers, the second being related to the first in some way. It finds
    those pairs of integers which are related to each other if the
    relation is transitive. It is supplied with,
    couples a matrix whose bound pairlist is [1:2, 1:number of
      identifier links] where couples [2, i] is related to couples
      [1, i] in some way.
    final linkage matrix a matrix whose bound pair list is
      [1:number of identifiers, 1:number of identifiers] and into
      which the procedure puts true if the second subscript
      expression is an integer which is related to the integer
      corresponding to the first subscript expression, if the
      relation is irreflexive then the diagonal entries of this
      matrix are false.
    iteration counter a place for the procedure to put the
      length of the longest chain it finds. CHAIN tracing can be
      applied to any system which can be represented by a Turing
      machine by letting the integers in couples correspond to
      the Turing machine states. Two integers j, k are related if
      there is an input symbol which causes state j to change to
      state k. If the Turing machine always stops whatever the
      sequence of input symbols, then its final linkage matrix
      will have false for all leading diagonal entries;
    integer i, j;
    Boolean array working linkage matrix [1:number of identi-
      fiers, 1:number of identifiers];
    Boolean procedure PROGRESS;
      begin PROGRESS := false;
        for i := 1 step 1 until number of identifiers
          do for j := 1 step 1 until number of identifiers
            do begin if Working linkage matrix [i, j] ≡ ¬ Final
                linkage matrix [i, j] then PROGRESS := true;
                Final linkage matrix [i, j] := Working linkage
                matrix [i, j]
              end of comparison
      end of PROGRESS;
BEGIN OF PROGRAM:
  for iteration counter := −1, 0, iteration counter + 1 while
      PROGRESS
    do for i := 1 step 1 until number of identifier links
      do for j := 1 step 1 until number of identifiers
        do begin if iteration number = −1
          thenFinal linkage Matrix [couples [1, i], j]
              := Working linkage Matrix [couples [1, i], j]
              := couples [2, i] = j
          else Working linkage Matrix [couples [1, i], j]
              := Working linkage Matrix [couples [1, i], j]
              ∨ Working linkage Matrix [couples [2, i], j];
          end of setting one linkage
end of CHAIN tracing;
```

ALGORITHM 70
INTERPOLATION BY AITKEN

CHARLES J. MIFSUD
General Electric Co., Bethesda, Md.

```
procedure AITKEN (x, f, n, X, F); real array x, f;
          integer n; real X, F;
comment If given x0 ,x1 , . . . xn , n+1 abscissas and also given
  f(x0), f(x1), . . . f(xn), n+1 functional values, this procedure
  generates a Lagrange polynomial, F(X) of the nth degree so that
  F(xi) = f(xi). Hence, for any given value X, a functional value
  F(X) is generated. The procedure is good for either equal or
  unequal intervals of the xi. Aitken's interative scheme is used
  in the generation of F(X). Since the f array is used for tem-
  porary storage, as the calculation proceeds its original values
  are destroyed;
begin integer i, j, t;
  for j := 0 step 1 until n−1 do
    begin t := j+1
      for i := t step 1 until n do
        f[i] := ((X−x [j]) × f [i] − (X−x [i]) × f[j])/
                (x[i] −x[j])    end
          F := f [n]
end
```

CERTIFICATION OF ALGORITHM 70
INTERPOLATION BY AITKEN [C. J. Mifsud, *Comm. ACM 4* (Nov. 1961)]

A. P. RELPH
The English Electric Co., Whetstone, England

Algorithm 70 was translated using the DEUCE ALGOL compiler and gave satisfactory results after semicolons had been added to

t := j+1 *to make it* t := j+1;

and (x[i]−x[j]) **end** *to make it* (x[i]−x[j]) **end**;

The identifier *t* can be eliminated and the algorithm shortened by the following changes:

Replace **begin integer** i, j, t; *by* **begin integer** i, j;
Replace t := j+1; **for** i := t **step** 1 **until** n **do** *by* **for** i := j+1 **step** 1 **until** n **do**

ALGORITHM 71
PERMUTATION

R. R. COVEYOU AND J. G. SULLIVAN
Oak Ridge National Laboratory, Oak Ridge, Tenn.

```
procedure PERMUTATION (I, P, N);
  value I, N; integer N; integer array P; boolean I;
  comment This procedure produces all permutations of the
    integers from 0 thru N. Upon entry with I = false the pro-
    cedure initializes itself producing no permutation. Upon each
    successive entry into the procedure with I = true a new
    permutation is stored in P[0] thru P[N]. When the process has
    been exhausted a sentinel is set:
    P[0] : −1,
    N ≥ 0;
  begin
    integer i; own integer array x[0:N];
    if ¬ I then
    begin for i := 0 step 1 until N−1 do x[i] := 0;  x[N] := −1;
      go to E end;
    for i := N step −1 until 0 do begin if x[i]≠i then go to A;
      x[i] := 0 end;
    P[0] := −1;  go to E;
A:  x[i] := x[i]+1;  P[0] := 0;
    for i := 1 step 1 until N do
      begin P[i] := P[i−x[i]];  P[i−x[i]] := i end;
E:  end PERMUTATION
```

CERTIFICATION OF ALGORITHM 71
PERMUTATION (R. R. Coveyou and J. G. Sullivan, *Comm. ACM*, Nov. 1961)

P. J. BROWN
University of North Carolina, Chapel Hill, N. C.

PERMUTATION was transliterated into GAT for the UNIVAC 1105 and successfully run for a number of cases.

CERTIFICATION OF ALGORITHM 71
PERMUTATION (R. R. Coveyou and J. G. Sullivan, *Comm. ACM*, Nov. 1961)

J. E. L. PECK AND G. F. SCHRACK
University of Alberta, Calgary, Alberta, Canada

PERMUTATION was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. The **own integer array** x[0:n] may be shortened to x[1:n], provided corresponding corrections are made in the first two **for** statements.

However, PERMUTE (Algorithm 86) is superior to PERMUTATION in two respects.

(1) PERMUTATION, using storage of order 2n, is designed to permute the specific vector 0, 1, 2, $\cdots$, n − 1 rather than an arbitrary vector. Thus storage of order 3n is required to permute an arbitrary vector. PERMUTE, in contrast, only needs storage of order 2n to permute an arbitrary vector.

(2) PERMUTE is built up from cyclic permutations. The number of permutations actually executed internally (the redundant ones are suppressed) by PERMUTE is asymptotic to (e − 1)n! rather than n!. In spite of this, PERMUTE is distinctly faster (1316 against 2823 seconds for n = 8) than PERMUTATION. If t_n is the time taken for all permutations of a vector with n components, and if $r_n = t_n/nt_{n-1}$, then one would expect r_n to be close to 1. Experiment with small values of n gave the following results for r_n.

n	6	7	8
PERMUTE	0.96	0.99	1.00
PERMUTATION	1.10	1.13	1.12

Is there yet a faster way to do it?

See also: C. Tompkins, "Machine Attacks on Problems whose Variables are Permutations", Proceedings of Symposia in Applied Mathematics, Vol. VI: *Numerical Analysis* (N. Y., McGraw-Hill, 1956).

CERTIFICATION OF ALGORITHM 71
PERMUTATION [R. R. Coveyou and J. G. Sullivan, *Comm. ACM*, Nov. 1961]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. The integer array x was made a parameter of the procedure in order to avoid having an **own** array with variable bounds.

ALGORITHM 72
COMPOSITION GENERATOR

L. HELLERMAN AND S. OGDEN
IBM-Product Development Laboratory, Poughkeepsie, N. Y.

```
procedure comp (c, k); value k; integer array c;
  integer k;
comment Given a k-part composition c of the positive integer n,
  comp generates a consequent composition if there is one. If
  comp operates on each consequent composition after it is found,
  all compositions will be generated, provided that 1, 1, . . ., 1,
  n−k+1 is the initial c. If c is of the form n−k+1, 1, 1, . . . , 1,
  there is no consequent, and c will be replaced by a k vector of
  0's. Reference: John Riordan, An Introduction to Combi-
  natorial Analysis, John Wiley and Sons, Inc., New York, 1958,
  Chapter 6;
begin integer j; integer array d [1:k];
  if k = 1 then go to last;
  for j := 1 step 1 until k do d [j] := c [j] − 1;
test: if d[j]>0 then go to set;
      j := j−1;
      go to if j = 1 then last else test;
set:  d [j] := 0;
      d [j − 1] := d [j − 1] + 1;
      d [k] := c [j] − 2;
      for j := 1 step 1 until k do c [j] := d[j] + 1;
      go to exit;
last: for j := 1 step 1 until k do c [j] := 0;
exit: end comp
```

CERTIFICATION OF ALGORITHM 72
COMPOSITION GENERATOR [L. Hellerman and S. Ogden, *Comm. ACM*, Nov. 1961]

D. M. COLLISON
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

After

```
for j := 1 step 1 until k do d[j] := c[j]−1;
```

the statement

```
j := k;
```

should be inserted (see ALGOL 60 report, para 4.6.5). With this alteration, the algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803.

ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS

DAVID K. JEFFERSON
U. S. Naval Weapons Laboratory, Dahlgren, Virginia

```
procedure ellint (k, phi, E, F);
value k, phi;
real phi, F, k, E;
comment ellint computes the value of the incomplete elliptic
    integrals of the first and second kinds, F(phi, k) and E(phi, k),
    where phi is in radians. If | k | > 1 or | phi | > π/2, E and F
    will be set equal to 100,000,000, otherwise they will contain the
    computed integrals. For the formulation of this procedure, see
    DiDonato, A. R., and Hershey, A. V., "New Formulae for
    Computing Incomplete Elliptic Integrals of the First and
    Second Kind", J. ACM 6, 4 (Oct. 1959);
begin real kp, sinphi, n, cosphi;
    real array H [1:2], A [1:2], sigma [1:4], L [1:2], M [1:2],
      N [1:2], T [1:2], del [1:4];
    sigma [1] := sigma [2] := sigma [3] := sigma [4] := 0;
    H [1] := 1;
    n := 0;
    sinphi := sin(phi);
if abs (k × sinphi) ≤ tanh (1) then go to small else if abs (k) ≤
    1 ∧ abs(phi) ≤ π/2 then go to large;
    E := F := 100000000;
    go to stop;
small: A [1] := phi;
step 1: n := n + 1;
    cosphi := cos (phi);
    E := (2 × n−1) /(2 × N);
    H [2] := E × k↑2 × H [1];
    A [2] := E × A [1] − sinphi ↑ (2 × n−1) × cosphi /(2 × n);
    del [1] := H [2] × A [2];
    del [2] := −k↑2 × H [1] × A [2] /(2 × n);
    sigma [1] := sigma [1] + del [1];
    sigma [2] := sigma [2] + del [2];
    H [1] := H [2];
    A [1] := A [2];
if abs ((sigma [1] + del [1]) − sigma [1]) > 0 ∧ phi × sinphi
    ↑ (2 × n) ≥ A [2] then go to step 1;
    F := phi + sigma [1];
    E := phi + sigma [2];
    go to stop;
large: kp := sqrt (1−k↑2);
    A [1] := 1;
    L [1] := M [1] := N [1] := 0;
step 2: n := n+1;
    E := (2 × n−1) /(2 × n);
    F := abs (k) × sqrt (1−sinphi ↑2) × (1−k↑2 × sinphi
      ↑2)↑((2 × n−1) /(2 × n));
    H [2] := E × H [1];
    A [2] := E↑2 × kp↑2 × A [1];
    L [2] := L [1] + 1 /(n × 2 × n−1));
M [2] := (M [1] − F × H [2]) × ((2 × n+1) /(2 × n+2))↑2 ×
    kp↑2;
N [2] := (N[1] − F × H [1]) × E × (2 × n+1) × kp↑2 /(2 ×
    n+2);
del [1] := M [2] − A [2] × L [2];
del [2] := N [2] − E × kp↑2 × A [1] × L [2] + kp↑2 × A [1]
    /((2 × n) ↑2);
del [3] := A [2];
del [4] := (2 × n+1) × A [2] /(2 × n+2);
sigma [1] := sigma [1] + del [1];
sigma [2] := sigma [2] + del [2];
sigma [3] := sigma [3] + del [3];
sigma [4] := sigma [4] + del [4];
H [1] := H [2];
A [1] := A [2];
L [1] := L [2];
M [1] := M [2];
N [1] := N [2];
if abs ((sigma [1] + del [1]) − sigma [1]) > 0 then go to step 2;
T [1] := ln (4 /(sqrt (1 − k↑2 × sinphi ↑2) + abs (k) × sqrt(1−
    sinphi ↑ 2)));
T [2] := abs (k) × sqrt ((1−sinphi ↑2) /(1−k↑2 × sinphi ↑2));
F := T [1] × (1+sigma [3]) + T [2] × ln (.5 + .5 × abs (k ×
    sinphi)) + sigma [1];
E := (.5 + sigma [4]) × kp↑2 × T [1] + 1−T [2] × (1−abs
    (k × sinphi)) + sigma [2];
stop: end
```

CERTIFICATION OF ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS (David K. Jefferson, *Comm. ACM*, Dec. 1961)

DEAN C. KRIEBEL
U. S. Naval Weapons Laboratory, Dahlgren, Virginia

This algorithm was originally coded in NORC machine language and K. Pearson's incomplete elliptic integral tables of the first and second kind generated. (See DiDonato, A. R., and Hershey, A. V., "New Formulae for Computing Incomplete Elliptic Integrals of the First and Second Kind", *J.ACM 6*, 4 (Oct. 1959)).

The algorithm was coded for the MAD Compiler exactly as written in ALGOL and run on an IBM 7090. Forty cases were computed with K ranging from 0° to 90° and PHI ranging from 0° to 90°. The results contained eight significant digits which agreed with the DiDonato and Hershey tables to within 0 to 2 units in the 8th digit. (This may be attributed to the decimal to binary, binary to decimal input-output conversion used with a binary computer as compared to straight decimal computation on the NORC.)

CERTIFICATION OF ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS [David K. Jefferson, *Comm. ACM 4*, Dec. 1961]

NOELLE A. MEYER
E. I. du Pont de Nemours & Co., Wilmington, Del.

Ellint was hand-coded in FORTRAN for the IBM 7070. The following corrections were made

The statement

$$E := (2\times n-1)/(2\times N);$$

should be

```
E := (2×n−1)/(2×n);
```

The statement

```
F := abs(k) × sqrt(1−sinphi ↑ 2) × (1−k ↑ 2×sinphi ↑ 2) ↑
                                        ((2×n−1)/(2×n));
```

should be

```
F := (abs(k)×sqrt(1−sinphi ↑ 2) ×
                (1−k ↑ 2×sinphi ↑ 2) ↑ (n−.5))/(2×n)
```

The statement

```
L[2] := L[1] + 1/(n×2×n−1));
```

should be

```
L[2] := L[1] + (1/(n×(2×n−1));
```

In order to accommodate negative ϕ the following changes were made:

The statement

```
if abs((sigma[1]+del[1])−sigma[1]) > 0 ∧ phi × sinphi ↑
                                    (2×n) ≥ A[2] then go to step 1;
```

was changed to

```
if abs((sigma[1]+del[1])−sigma[1])>0∧abs(phi×sinphi ↑ (2×n))
                                    ≥ abs(A[2]) then go to step 1;
```

Also the following was inserted before the last statement (*stop*: **end**)

```
        if phi < 0 then go to wait else go to stop;
wait:   F := −F;
        E := −E;
```

The revised algorithm yielded satisfactory answers when compared with the DiDonato and Hershey tables. Differences occurred in the eighth significant digit as shown in the following difference tables.

DIFFERENCE TABLES

F-TABLE

ϕ (in degrees) \ θ (in degrees)	0	30	60	90
0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-3×10^{-8}
60	1×10^{-8}	1×10^{-8}	2×10^{-8}	-3×10^{-8}
90	0.	2×10^{-8}	6×10^{-8}	0.

E-TABLE

0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}
60	1×10^{-8}	1×10^{-8}	-7×10^{-8}	3×10^{-8}
90	0.	0.	1×10^{-8}	0.

CERTIFICATION OF ALGORITHM 73 INCOMPLETE ELLIPTIC INTEGRALS [David K Jefferson, *Comm. ACM* Dec. 1961]

R. P. VAN DE RIET
Mathematical Centre, Amsterdam

The algorithm contained three misprints:

The 26th line of the procedure

```
E := (2 × n−1)/(2 × N);
```

should read

```
E := (2 × n−1)/(2 × n);
```

The 46th line of the procedure

```
↑ 2) ↑ ((2 × n−1)/(2 × n));
```

should read

```
↑ 2) ↑ ((2 × n−1)/2)/(2 × n);
```

The 49th line of the procedure

```
L [2] := L [4] + 1/(n × 2 × n−1));
```

should read

```
L [2] := L [1] + 1/(n × (2 × n−1));
```

The program was run on the X1 computer of the Mathematical Centre. For *phi* = 45°, *k* = *sin*(10°(10°)180°), *E* and *F* were calculated. The result contained 12 significant digits.

Comparison with a 12-decimal table of Legendre-Emde (1931) showed that the 12th digit was affected with an error, at most 4 units large. After about 10 minutes of calculation (i.e. more than 100 cycles) no results were obtained for *k* = *sin* 89°, *phi* = 1° and the calculation was discontinued.

REMARKS. As *phi* is unchanged during the calculation, we placed the statement *cos phi* := *cos* (*phi*) in the beginning of the program, to be certain that the cosine was not calculated 30 or more times. Moreover, in the expression for *T*[1] and *T*[2], *sqrt* (1-*sin phi* ↑ 2) was replaced by *cos phi*, so that loss of significant figures does not occur.

The expression $2 \times n$ was changed in a new variable, to obtain a more rapid program.

REMARK ON ALGORITHM 73 INCOMPLETE ELLIPTIC INTEGRALS [David K. Jefferson, *Comm. ACM* (Dec. 1961)]

DAVID K. JEFFERSON
U. S. Naval Weapons Laboratory, Dahlgren, Virginia

In regard to Algorithm 73, two errors were found:

The 34th line of the procedure

```
F := abs(k) × sqrt (1−sinphi ↑ 2)
    × (1−k ↑ 2 × sinphi ↑ 2) ↑ ((2 × n−1)/(2 × n));
```

should read

```
F := abs(k) × sqrt (1−sinphi ↑ 2)
  × (1−k ↑ 2 × sinphi ↑ 2) ↑ ((2 × n−1)/2)/(2 × n);
```

The 37th line

```
L[2] := L[1] + 1/(n × 2 × n−1));
```

should read

```
L[2] := L[1] + 1/(n × (2 × n−1));
```

In addition, efficiency is improved by interchanging lines 13 and 14:

```
Step 1:  n := n+1;
         cosphi := cos(phi);
```

can be replaced by

```
         cosphi:=cos(phi);
Step 1:  n := n + 1;
```

ALGORITHM 74

CURVE FITTING WITH CONSTRAINTS

J. E. L. PECK,
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```
procedure Curve fitting (k,a,b,m,x,y,w,n,alpha,beta,s,sgmsq,x0,
  gamma,c,z,r);
comment This procedure finds, by the method of least squares,
  the polynomial of degree n, k ≤ n < k+m, whose graph con-
  tains (a1 , b1), ··· , (akbk) and approximates (x1 , y1), ··· ,
  (xm, ym), where wi is the weight attached to the point (xi , yi).
  The details will be found in the reference cited below, where a
  similar notation is used. A nonlocal label "error" is assumed;
  value a, x, y, w; integer k, m, n, r; real x0, gamma; array
    a, b, x, y, w, alpha, beta, s, sgmsq, c, z;
  begin integer i,,j; array w1[1:k]; real p, f, lambda;
  comment We shall first define several procedures to be used
    in the main program, which begins at the label START;

procedure Evalue (x, nu);
comment This procedure evaluates f = s0p0 + s1p1 + ··· +
  snpn , where p-1(x) = 0, p0(x) = 1, β0 = 0 and pi+1(x)
  = (x − αi)pi(x) − βipi-1(x), i = 0, 1, ··· , ν−1. The value of
  pν(x) remains in p;
  real x; integer nu;
  begin real p0, temp; integer i; p0 := 0; p := 1; f := s[0];
for i := 0 step 1 until nu−1 do
  begin temp := p;
  p := (x−alpha[i]) × p−beta[i] × p0;
  p0 := temp; f := f + p × s[i+1] end i
end Evalue;

procedure Coda (n, c);
comment This procedure finds the c's when c0 + c1x + ··· +
  cnxn = s0p0(x) + ··· + snpn(x);
  integer n; array c;
  begin integer i,r; real t1,t2; array pm,p[0:n];
for r := 1 step 1 until n do
  c[r] := pm[r] := p[r] := 0;
pm[0] := 0; p[0] := 1; c[0] := s[0];
for i := 0 step 1 until n−1 do
  begin t2 := 0;
  for r := 0 step 1 until i+1 do
    begin t1 := (t2−alpha[i] × p[r]−beta[i] × pm[r])/lambda;
    t2 := pm[r] := p[r]; p[r] := t1;
    c[r] := c[r] + t1 × s[i+1]end r
  end i
end Coda;

procedure GEFYT (n,n0,x,y,w,m);
comment This is the heart of the main program. It computes
  the αi,βi,si,σi², using the method of orthogonal polynomials, as
  described in the reference;
  integer n,n0,m; array x,y,w;
  begin real dsq,wpp,wpp0,wxpp,wyp,temp;
integer i,j,freedom; array p,p0[1:m]; boolean exact;
if n−n0 > m ∨ n < n0 then go to error;
beta[n0] := dsq := wpp := 0; exact := n−n0 ≥ m−1;
for j := 1 step 1 until m do
  begin p[j] := 1; p0[j] := 0; wpp := wpp + w[j];
  if ¬ exact then dsq := dsq + w[j] × y[j] × y[j] end initialise;
for i := n0 step 1 until n do
  begin freedom := m−1−(i−n0); wyp := wxpp := 0;
  for j := 1 step 1 until m do
    begin temp := w[j] × p[j];
    if i < n then wxpp := wxpp + temp × x[j] × p[j];
    if freedom ≥ 0 then wyp := wyp + temp × y[j] end j;
  if freedom ≥ 0 then s[i] := wyp/wpp;
  if ¬ exact then begin dsq := dsq − s[i] × s[i] × wpp;
  sgmsq[i] := dsq/freedom end if;
  if i < n then begin alpha[i] := wxpp/wpp; wpp0 := wpp;
  wpp := 0;
  for j := 1 step 1 until m do
    begin temp := (x[j]−alpha[i]) × p[j] − beta[i] × p0[j];
    wpp := wpp + w[j] × temp × temp;
    p0[j] := p[j]; p[j] := temp end j;
  beta[i+1] := wpp/wpp0 end if
  end i
end GEFYT;
    START: for j := 1 step 1 until k do
begin w1[j] := 1; a[j] = (a[j]−x0)/gamma end j;
GEFYT (k,0,a,b,w1,k);
comment This finds the polynomial of degree k−1 whose graph
  contains (a1,b1),···,(ak,bk) supplying the αi,βi,si, 0 ≤ i ≤ k;
  begin real rho; rho := 0;
for j := 1 step 1 until m do
  begin rho := rho + w[j];
  x[j] := (x[j] − x0)/gamma end j; rho := m/rho;
comment The factor ρ is used to normalize the weights. We shall
  now put sk = 0 in order to evaluate pk(x) and the polynomial of
  degree k−1 simultaneously;
s[k] := 0;
for j := 1 step 1 until m do
  begin Evalue (x[j],k);
  if p = 0 then go to error;
  y[j] := (y[j] − f)/p;
  w[j] := w[j] × p × p × rho end j
end rho;
comment We have now normalized the weights and adjusted
  the weights and ordinates ready for the least squares approxi-
  mation;
GEFYT (n,k,x,y,w,m);
comment The coefficients αi,βi, 0 ≤ i < n, and si, 0 ≤ i ≤ n
  are now ready. The polynomial may be evaluated for x = z1,z2,
  ···,zr, but the variable must be adjusted first. Note that we
  may evaluate the best polynomial of lower degree by decreas-
  ing n;
  begin real x;
for j := 1 step 1 until r do
  begin x := (z[j]−x0)/gamma;
  Evalue (x,n); comment the values of zj and f should now be
    printed; end j;
comment We may now adjust the coefficients for scale and then
  find the coefficients of the power series c0 + c1x + ··· + cnxn =
  s0p0(x) + ··· + snpn(x);
for i := 0 step 1 until n−1 do
  begin alpha[i] := alpha[i] × gamma + x0;
  beta[i] := beta[i] × gamma end i; lambda := gamma;
Coda (n,c);
comment We may now re-evaluate the polynomial from the
  power series;
for j := 1 step 1 until r do
```

```
  begin x := z[j];  f := c[n];
  for i := n−1 step −1 until 0 do
    f := f × x + c[i];
  comment  the values of x and f should now be printed;  end j
  end x
end Curve fitting
```

REFERENCE: PECK, J. E. L. Polynomial curve fitting with constraint, *Soc. Indust. Appl. Math. Rev.* (1961).

CERTIFICATION OF ALGORITHM 74 CURVE FITTING WITH CONSTRAINTS [J. E. Peck, *Comm. ACM*, Jan. 62]

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Algorithm 74 was hand-compiled into SOAP IIa for the IBM 650 and run successfully with no corrections except the case in which the origin (0, 0) are given as both a constraint and a sample.

ALGORITHM 75
FACTORS

J. E. L. PECK,
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```
procedure factors (n,a,u,v,r,c);
comment This procedure finds all the rational linear factors of
  the polynomial a0x^n + a1x^(n-1) + ... + a(n-1)x + an, with integral
  coefficients. An absolute value procedure abs is assumed;
value n,a; integer r,n,c; integer array a,u,v;
begin comment We find whether p divides a0, 1 ≤ p ≤ |a0| and
  q divides an, 0 ≤ q ≤ |an|. If this is the case we try (px ± q);
integer p,q,a0,an;
r := 0; c := 1; comment r will be the number of linear factors
  and c the common constant factor;
TRY AGAIN: a0 := a[0]; an := a[n];
for p := 1 step 1 until abs(a0) do
  begin if (a0 ÷ p) × p = a0 then
    begin comment p divides a0;
    for q := 0 step 1 until abs(an) do
      begin if q = 0 ∨ (an ÷ q) × q = an then
        begin comment q divides an (or q = 0). If p = q we
          may have a common constant factor, therefore; if q
          > 1 ∧ p = 1 then
          begin integer j;
          for j := 1 step 1 until n-1 do
            if (a[j] ÷ q) × q ≠ a[j] then go to NO CONSTANT;
          for j := 0 step 1 until n do
            a[j] := a[j]/q;
          c := c × q; go to TRY AGAIN
          end the search for a common constant factor;
        NO CONSTANT:
          begin comment try (px - q) as a factor;
          integer f,g,i; f := a0; g := 1;
          comment we try x = q/p;
          for i := 1 step 1 until n do
            begin g := g × p; f := f × q + a[i] × g
            end evaluation;
          if f = 0 then
            begin comment we have found the factor (px - q);
            r := r + 1; u[r] := p; v[r] := q;
            comment there are now r linear factors;
              begin comment we divide by (px - q);
              integer i,t; t := 0;
              for i := 0 step 1 until n do
                begin a[i] := t := (a[i] + t)/p; t := t × q
                end i;
              n := n - 1
              end reduction of polynomial. Therefore;
            go to if n = 0 then REDUCED else TRY AGAIN
            end discovery of px - q as a factor. But
          if we got this far it was not a factor so try px + q;
          q := -q; if q < 0 then go to NO CONSTANT
          end trial of px ± q,
        end q divides an and
      end of q loop.
    end p divides a0, also
    end p loop, which means;
REDUCED: if n = 0 then
    begin c := c × a0; a0 := 1
    end if n = 0
end factors procedure. There are now r (r > 0) rational linear
  factors (uix - vi), 1 < i < r, and the reduced polynomial of
  reduced degree n replaces the original. The common constant
  factor is c. Acknowledgments to Clay Perry.
```

CERTIFICATION OF ALGORITHM 75
FACTORS [J. E. L. Peck, *Comm. ACM 5* (Jan. 1962)]

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Algorithm 75 was translated using the DEUCE ALGOL compiler and gave satisfactory results after the following corrections had been made:

```
    begin if q=0∨(an÷q)×q=an then
      begin if q>1∧p=1 then
was changed to
    begin if q≦1 then go to NO CONSTANT;
      if (an÷q)×q=an then
      begin if p=q then

    begin c := c×a0; a0 := 1
    end
was changed to
    begin c := c×a[0]; a[0] := 1;
    end
```

There are now r (r>0) rational linear factors (u i x−vi), 1<i<r,

was changed to

If r>0 there are now r rational linear factors (uix−vi), 1≦i≦r,

CERTIFICATION OF ALGORITHM 75
FACTORS [J. E. L. Peck, *Comm. ACM*, Jan. 1962]

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The following changes had to be made to the algorithm:

(1) *For* **if** $q > 1 \wedge p = 1$ **then**
put **if** $q > 1 \wedge p = q$ **then**

(2) *For* **begin** $c := c \times a0$; $a0 := 1$ **end**
put **begin** $c := c \times a[0]$; $a[0] := 1$ **end**

(3) *For* **if** $q = 0 \vee (an \div q) \times q = an$ **then**
put **if (if** $q = 0$ **then true else** $(an \div q) \times q = an$**) then**

This change is necessary to ensure that the term $(an \div q)$ is not evaluated when $q = 0$.

The algorithm, thus modified, was successfully run using the Elliott ALGOL translator on the National-Elliott 803.

To return to the state ($p=1$, $q=0$) after every factor or constant is found is inefficient. This can be avoided by substituting a[0] and a[n] for the identifiers a0 and an respectively. The procedure then becomes:

```
procedure factors (n, a, u, v, r, c); value n, a;
  integer array a, u, v;
integer r, n, c;
begin integer p, q;
  r := 0;  c := 1;
ZERO:  if a[n]=0 then
         begin r := r+1;  u[r] := 1;  v[r] := 0;  n := n-1;
           go to ZERO
         end;
         for p := 1 step 1 until abs (a[0]) do
         begin if (a[0]÷p)×p=a[0] then
           begin for q := 1 step 1 until abs (a[n]) do
             begin if q=1 then go to NO CONSTANT;
           TRY AGAIN:  if (a[n]÷q)×q=a[n] then
                       begin integer j;
                         for j := 0 step 1 until n-1 do
                           if (a[j]÷q)×q≠a[j] then go to
                           NO CONSTANT;
                         for j := 0 step 1 until n do
                           a[j] := a[j]/q;
                         c := c×q;  go to TRY AGAIN
                       end;
       NO CONSTANT:  begin integer f, g, i;  f := a[0];
                       g := 1;
                       for i := 1 step 1 until n do
                       begin g := g×p;
                         f := f×q+a[i]×g
                       end;
                       if f=0 then
                       begin r := r+1;  u[r] := p;
                         v[r] := q;
                         begin integer i, t;  t := 0;
                           for i := 0 step 1 until n do
                           begin a[i] := t := (a[i]+t)/p;
                             t := t×q
                           end;
                           n := n-1
                         end
                         go to if n=0 then REDUCED
                           else NO CONSTANT
                       end;
                       q := -q;  if q<0 then go to NO
                         CONSTANT
                     end
           end
         end
       end;
       REDUCED:  if n=0 then
         begin c := c×a[0];  a[0] := 1
         end
end
```

ALGORITHM 76
SORTING PROCEDURES

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comment The following ALGOL 60 algorithms are procedures for the sorting of records stored within the memory of the computer. These procedures are described in detail, flow-charted, compared, and contrasted in "Analysis of Internal Computer Sorting" by Ivan Flores [*J. ACM 8* (Jan. 1961)]. Although sorting is usually a business computer application, it can be described completely in ALGOL if we stretch our imagination a little. Sorting is ordering with respect to a key contained within the record. If the key *is* the active record, the sorting is trivial. A means is required to extract the key from the record. This is essentially string manipulation, for which no provision, as yet, has been made in ALGOL. We circumambulate this difficulty by defining an **integer procedure** K(I) which "creates" a key from the record, I. ALGOL *does* provide for machine language code substitutions, which is one way to think of K(I). This could be more accurately represented by using the string notation proposed by Julien Green ["Remarks on ALGOL and Symbol Manipulation," *Comm. ACM 2* (Sept. 1959), 25–27]. The function **sub** ($,i,g) represents the procedure, K(I). $ corresponds to the record I, i corresponds to the starting position of the key and g corresponds to the length of the key. Both i and g are **values** which must be specified when the sort procedure is called for as a statement instead of a declaration.

Another factor, which might vex some, is that the key might be alphabetic instead of numeric. Then, of course, K(I) would not be integer. It would, however, be string when such is defined eventually. Note, also, that keys are frequently compared. This is done using the ordering relations ">" for "greater than," etc. These are not really defined in the ALGOL statement [NAUR, PETER, ET AL. "Report on the Algorithmic Language ALGOL 60". *Comm. ACM 3* (May 1960), 294–314]. They can simply be defined so that $Z > Y > \cdots > A > 9 > \cdots > 1 > 0$. Also the assignment X[i] := z should be interpreted as "Assign the key 'z' which is larger than any other key." For any sort procedure (I,N,S), "I" is the set of unsorted records, "N" is their number, and "S" the sorted set of records.

Caution, these algorithms were developed purely for the love of it: No one was available with the combined knowledge of sorting and ALGOL to check this work. Hence each algorithm should be carefully checked before use. I will be glad to answer any questions which may arise;

```
Sort insert (I,N,S); value N; array I[1:N], S[1:N];
  integer procedure K(I); integer N;
  begin integer i, j, k;
    S[1] := I[1];
    for i := 2 step 1 until N do begin
      for j := i − 1, j − 1 while K(I[i]) > K(S[j]) do
      for k := i step − 1 until j + 1 do
        S[k] := S[K − 1];
      S[j + 1] := I[i] end end
```

```
Sort count (I,N,S); value N; array I[1:N], S[1:N];
  integer procedure K(I); integer N;
  begin integer array C[1:N]; integer i,j;
    for i := 1 step 1 until N do C[i] := 0;
    for i := 2 step 1 until N do
      for j := 1 step 1 until i − 1 do
        if K(I[i]) > K(I[j]) then C[i] := C[i] + 1
        else C[j] := C[j] + 1;
    for i := 1 step 1 until N do
      S[C[i]] := I[i] end
```

```
Sort select (I,N,S); value N; array I[1:N], S[1:N];
  integer procedure K(I); integer N;
  begin integer i,j,A,h;
    for i := 1 step 1 until N do begin
    h := K(I[1]);
    for j := 2 step 1 until N do
    if h > K(I[j]) then begin h := K(I[j]); A := j end;
    S[i] := I[A];
    I[A] := z end end
```

```
Sort select exchange (I,N); value N; array I[1:N];
  integer procedure K(I); integer N;
  begin integer h,i,j,H; real T;
    for i := 1 step 1 until N do begin
      H := K(I[i]); h := i;
      for j := i + 1 step 1 until N do
        if K(I[j]) < H then begin
        H := K(I[j]); h := j end
      T := I[i]; I[i] := I[h]; I[A] := T end
  end
```

```
Sort binary insert (I,N,S); value N; array I[1:N], S[1:N];
  integer procedure K(I); integer N;
  begin integer i,k,j,l;
    if K(I[1]) < K(I[2]) then begin
      S[1] := I[1]; S[2] := I[2] end
      else begin S[1] := I[2]; S[2] := I[1] end;
  start:  for   i := 3 step 1 until N do begin
                j := (i + 1) ÷ 2;
  find spot:    for k := (i + 1) ÷ 2, (k + 1) ÷ 2 while k > 1 do
                  if K(I[i]) < K(S[j]) then j := j − k
                  else j := j + k;
                if K(I[i]) ≥ K(S[j]) then j := j − 1;
  move items:   for l := i step − 1 until j do
                  S[l + 1] := S[l];
  enter this
  one:          S[j] := I[i] end end
```

```
Sort address calculation (I,N,S,F); value N;
  array S[1:M], I[1:N]; integer procedure F(K), K(I);
  integer N,M;
            begin integer i,j,G,H,F,M;
              M := entier(2.5 × N)
              for i := 1 step 1 until M do S[i] = 0;
  Address:    for i := 1 step 1 until N do begin
              F := F(K(I[i]));
              if S[F] = 0 then begin S[F] := I[i];
                go to NEXT end
              else if K(S[F]) > K(I[i]) then go to SMALLER;
  LARGER:     for H := F, H + 1 while K(S[H]) < K(I[i]) do
              for G := H, G + 1 while K(S[G]) ≠ 0 do
              for j := G step −1 until H + 1 do
                S[j] := S[j − 1];
              S[H] := I[i]; go to NEXT;
  SMALLER:    for H := F, H − 1 while K(S[H]) > K(I[i]) do
```

```
            for G := H, G − 1 while K(S[G]) ≠ 0 do
            for j := G step 1 until H − 1 do
              S[j] = S[j + 1];
            S[H] := I[i];
NEXT:     end end
```

```
Sort quadratic select (I,N,S); value N; array I[1:N], S[1:N];
  integer procedure K(I); integer N;
              begin integer i,j,k,C,D,J,M;
                integer array C[1:M], D[1:M];
                array I[1:M, 1:M];
  Divide inputs: M := entier (sqrt (N)) + 1; j := k := 1;
              for i := 1 step 1 until N do begin
                I[j,k] := I[i]; k := k + 1;
                if k > M then begin k := 1;
                  j := j + 1 end end
  Fill up inputs: I[j,k] := z; k := k + 1;
              if k > M then begin k := 1; j := j + 1 end
              if j ≤ M then go to Fill up inputs;
  Set controls: for j := 1 step 1 until M do begin
              C[j] := K(I[j, 1]); D[j] := 1;
              for k = 2 step 1 until M do
                if C[j] > K(I[j,k]) then begin
                C[j] := K(I[j,k]); D[j] := k end end;
              i := 1;
  Find least: C := C[1]; D := D[1]; J := 1;
              for j := 2 step 1 until M do
                if C > C[j] then begin C := C[j];
                  D := D[j]; J := j end;
  Fill file:  S[i] := I[J,D]; i := i + 1; I[J,D] := z;
              if i = N + 1 go to STOP;
  Reset controls: for j := J do begin
              C[j] := K(I[j, 1]); D[j] := 1;
              for k := 2 step 1 until M do
                if C[j] > K(I[j,k]) then begin C[j] :=
                  K(I[j,k]; D[j] := k end end;
              go to Find least;
  STOP:       end
```

```
Presort quadratic selection (I,N,S); value N;
  array I[1:N], S[1:N]; integer procedure K(I); integer N;
              begin integer i,j,k,C,J,M;
                integer array C[1:M], D[1:M];
                  array I[1:M,1:M];
  Divide inputs: M := entier (sqrt(N)) + 1; j := k := 1;
              for i := 1 step 1 until N do begin
                I[j,k] := I[i]; k := k + 1;
                if k > M then begin k := 1;
                  j := j + 1 end end
  Fill up inputs: I[j,k] := z; k := k + 1;
              if k > M then begin k := 1; j = j + 1 end
              if j ≤ M then go to Fill up inputs;
  First sort: for j := 1 step 1 until M do
              sort select exchange (I[j,k],M);
  Set controls: for j := 1 step 1 until M do begin
                C[j] := K(I[j,1]); D[j] := 1 end
              i := 1;
  Find least: C := C[1]; J := 1;
              for j := 1 step 1 until M do
                if C > C[j] then begin C := C[j];
                  J := j end;
  Fill file:  S[i] := I[J,D[J]]; i := i + 1;
              if i = N + 1 go to STOP
  Reset control: for j := J do begin
                D[j] := D[j] + 1;
                if D[j] > M then C[j] := z else C[j] :=
                  K(I[j, D[j]]) end
              go to Find least;
  STOP:       end
```

```
Sort binary merge (I,N,S); value N; array I[1:N];
  integer procedure K(I); integer N;
  begin real array S[1:N];
  integer array A[0:1, 0:J[a]], B[0:1, 0:K[b]], Aloc[0:1, 0:J[a]],
    Bloc[0:1, 0:K[b]], J[0:1], K[0:1], j[0:1], k[0:1];
    integer a,b,i,j,k;
  distribute:   a := b := j[0] := j[1] := 1;
                for i := 1 step 1 until N do begin
                  if K(I[i]) < K(I[i−1] then
                    if a = 1 then a := 0 else a := 1;
                  A[a, j[a]] := K(I[i]); Aloc[a, j[a]] := i;
                    j[a] := j[a] + 1 end;
                J[0] := j[0]; J[1] := j[1];
  next sort:    begin a := b := j[0] := j[1] := k[0] :=
                  k[1] := 1;
  two inputs:   if A[1, j[1]] ≤ A[0, j[0]] then a := 1 else
                  a := 0;
                B[b, k[b]] := A[a, j[a]];
                  Bloc[b, k[b]] := Aloc[a, j[a]];
                j[a] := j[a] + 1; k[b] := k[b] + 1;
                if A[a, j[a]] ≥ A[a, j[a] − 1] then go to two
                  inputs else
                if a = 1 then a := 0 else a := 1;
  single step:  B[b, k[b]] := A[a, j[a]];
                  Bloc[b, k[b]] := Aloc[a, j[a]];
                j[a] := j[a] +1; k[b] := k[b] + 1;
                if A[a, j[a]] ≥ A[a, j[a] − 1] then go to
                  single step;
  switch file:  if b = 1 then b := 0 else b := 1;
  check rollout: for a := 0, 1 do
                  if j[a] = J[a] then go to rollout;
                go to two inputs;
  rollout:      B[b, k[b]] := A[a, j[a]];
                  Bloc[b, k[b]] := Aloc [a, j[a]];
                k[b] := k[b] + 1; j[a] := j[a] + 1;
                if j[a] = J[a] then go to interchange files;
                if A[a, j[a]] < A[a, j[a] − 1] then
                  if b = 1 then b := 0 else b := 1;
                go to rollout;
  interchange files: K[0] := k[0]; K[1] := k[1];
                if K[0] = 1 then go to output end
                for b := 1, 0 do begin
                  for k[b] := 1 step 1 until K[b] do begin
                    A[b, k[b]] := B[b, k[b]];
                      Aloc[b, k[b]] := Bloc[b, k[b]];
                    J[b] := K[b] end end
                go to next sort;
  output:       for i := 1 step 1 until N do
                    S[i] := I[Bloc[0, i]];
                end
```

REMARK ON ALGORITHM 76
SORTING PROCEDURES (Ivan Flores, *Comm. ACM 5*, Jan. 1962)

B. RANDELL
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The following types of errors have been found in the Sorting

Procedures:

1. Procedure declarations not starting with **procedure**.
2. Bound pair list given with array specification.
3. = used instead of :=, in assignment statements, and in a **for** clause.
4. A large number of semicolons missing (usually after **end**).
5. Expressions in bound pair lists in array declarations depending on local variables.
6. Right parentheses missing in some procedure statements.
7. Conditional statement following a **then.**
8. No declarations for A, or z, which is presumably a misprint.
9. In several procedures attempt is made to use the same identifier for two different quantities, and sometimes to declare an identifier twice in the same block head.
10. In the Presort quadratic selection procedure an array, declared as having two dimensions, is used by a subscripted variable with only one subscript.
11. At one point a subscripted variable is given as an actual parameter corresponding to a formal parameter specified as an array.
12. In several of the procedures, identifiers used as formal parameters are redeclared, and still assumed to be available as parameters.
13. In every procedure K is given in the specification part, with a parameter, whilst not given in the formal parameter list.

No attempt has been made to translate, or even to understand the logic of these procedures. Indeed it is felt that such a grossly inaccurate attempt at ALGOL should never have appeared as an algorithm in the *Communications*.

ALGORITHM 77
INTERPOLATION, DIFFERENTIATION, AND INTEGRATION

PAUL E. HENNION

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```
real procedure  AVINT (nop, jt, xarg, xlo, xup, xa, ya);
                value nop, jt, xarg, xlo, xup; real xarg, xlo, xup;
                integer nop, jt; real array xa, ya;
```

comment This procedure will perform interpolation, differentiation, or integration operating upon functions of one variable which over part or all of the interval of interest are adequately described by a di-parabolic fit.

The routine was originally programmed as an open subroutine for the IBM 704 in FORTRAN II and occupied 323 memory locations. It is based upon a Lagrange interpolation scheme specialized for averaged second order parabolas. The technique finds the slope of a function numerically defined at points 1, 2, 3 and 4 by fitting a parabola through the points 1, 2, 3, and another parabola through the points 2, 3, and 4. The slope then, at point 2, is the average analytical derivative of the two parabolas, i.e. the coefficients of the parabola through points 1, 2 and 3 ($a_1x_2^2+b_1x_2+c_1$) and the coefficients of the parabola through points 2, 3, and 4 ($a_2x_2^2+b_2x_2+c_2$) are determined by applying Lagrange's equations as shown below. The arithmetic mean of these coefficients $a = (a_1+a_2)/2$, $b = (b_1+b_2)/2$, $c = (c_1+c_2)/2$ are used to supply the slope in the interval from 2 to 3, namely $(2ax + b)$.

The interpolation is calculated in similar fashion, except the final formula is that a parabola $(ax^2 + bx + c)$.

The integration is performed likewise by a curve fitting process, e.g. the integral between any two points say 2 and 3 is the average integral of the two parabolas between the independent coordinate limits for points 2 and 3. The averaging process is done for each interval along the abscissa as the results obtained are accumulated to evaluate the definite integral.

Applying Lagrange's equations, the coefficients a, b, and c may be found by defining: $T_j = y_j/\prod_{i=1,\, i\neq j}^{n} (X_j - X_i)$ where $y = f(x)$, $n = 3$, $j = 1, 2, \cdots, n$, then $a = \sum_{i=1}^{n} T_i$, $b = \sum_{i=1}^{n} T_i \sum_{j=1,\, j\neq i}^{n} X_j$, $c = \sum_{i=1}^{n} T_i \prod_{j=1,\, j\neq i}^{n} X_j$;

```
begin real  ca, cb, cc, a, b, c, syl, syu, term1, term2, term3, da,
              dif, sum;
integer     jm, js, jul, ia, ib;
    start:  switch alpha := L1, L1, L12; switch beta := L9,
              L5, L6;
            switch gamma := L10, L11; switch delta := L8,
              L8, L13;
comment     For interpolation, differentiation or integration set
              jt = 1, 2, or 3 respectively;
            go to alpha [jt];
    L1:     if xarg ≥ xa [nop] then go to L2;
            if xarg ≥ xa [nop−1] then go to L2;
            if xarg ≤ xa [1] then go to L3;
            if xarg ≤ xa [2] then go to L3; go to L4;
    L2:     jm := nop−1; js := 1; go to term;
    L3:     jm := 2; js := 1; go to term;
comment     Locate argument;
    L4:     for ia := 2 step 1 until nop do begin
            if xa [ia] > xarg then go to L7; jm := ia end;
comment     Before loop is complete xarg ≤ xa [ia];
    L5:     ca := a; cb := b; cc := c; js := 3; im :=
              jm+1; go to term;
    L6:     a := (ca+a)/2; b := (cb+b)/2; c := (cc+c)/2;
              go to L9;
    L7:     js := 2; go to term;
    L8:     go to beta [js];
    L9:     go to gamma [jt];
comment     Interpolation, jt = 1;
    L10:    da := a × xarg ↑ 2 + b × xarg + c; go to exit1;
comment     Differentiation, jt = 2;
    L11:    dif := 2 × xarg + b; go to exit2;
comment     Integration, jt = 3;
    L12:    sum := 0; syl := xlo; jul := nop − 1;
              ib := 2;
    L16:    for jm := ib step 1 until jul do begin;
comment     Lagrange formulae;
            term1 := ya [jm − 1]/((xa [jm − 1] − xa[jm]) ×
              (xa[jm − 1] − xa[jm + 1]));
            term2 := ya [jm]/((xa [jm] − xa [jm − 1]) ×
              (xa[jm] − xa [jm + 1]));
            term3 := ya [jm + 1]/((xa [jm + 1] − xa [jm − 1]) ×
              (xa [jm + 1] − xa [jm]));
            a := term1 + term2 + term3;
            b := −(xa [jm] + xa [jm + 1]) × term1 − (xa
              [jm − 1] + xa [jm + 1]) × term2 − (xa [jm − 1] +
              xa [jm]) × term3;
            c := xa [jm] × xa [jm + 1] × term1 + xa [jm − 1] ×
              xa [jm + 1] × term2 + xa [jm − 1] × xa [jm] ×
              term3; go to delta [jt];
    L13:    if jm ≠ 2 then go to L14;
            ca := a; cb := b; cc := c; go to L15;
    L14:    ca := (a + ca)/2; cb := (b + cb)/2; cc :=
              (c + cc)/2;
    L15:    syu := xa [jm];
            sum := sum + ca × (syu ↑ 3 − syl ↑ 3)/3 + cb ×
              (syu ↑ 2 − syl ↑ 2)/2 + cc × (syu − syl);
            ca := a; cb := b; cc := c; syl := syu end;
comment     End of loop on [jm] index;
            sum := sum + ca × (xup ↑ 3-syl ↑ 3)/3 + cb ×
              (xup ↑ 2-syl ↑ 2)/2 + cc × (xup − syl); go
              to exit3;
    term:   ib := jm; jul := ib; go to L16;
comment     The results for interpolation, differentiation, and
              integration are da, dif, and sum respectively;
    exit1:  AVINT := da; go to exit;
    exit2:  AVINT := dif; go to exit;
    exit3:  AVINT := sum;
    exit:   end
```

CERTIFICATION OF ALGORITHM 77
AVINT (Paul E. Hennion, *Comm. ACM 5*, Feb., 1962)

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AVINT was transliterated into BAC-220 (a dialect of ALGOL-58) and was tested on the Burroughs 220 computer. The following minor errors were found:

1. The first statement following label L11 should read:
   dif := 2 × a × xarg + b;
2. The semicolon (;) at the end of the line beginning with the label L16 should be deleted.
3. There appears to be a confusion between "1" (numeric) and "l" (alphabetic) following label L12. This portion of the program should read:
   L12: sum := 0; syl := xlo; jul := nop − 1; ib := 2;

After making the above corrections the procedure was tested for interpolation, differentiation, and integration using e^x, log X, and sin X in the range ($1.0 \leqq X \leqq 5.0$). Twenty-one values of each of these functions, evenly spaced with respect to X and accurate to at least 7 significant digits, were tabulated in the above range. Then the procedure was tested. The following table indicates approximately the accuracy obtained:

	Number of Significant Digits		
Function	*Interpolation*	*Differentiation*	*Integration*
e^x	$\geqq 4$*	$\geqq 2$	$\geqq 4$
log X	$\geqq 4$*	$\geqq 2$	$\geqq 3$
sin X	$\geqq 4$*	$\geqq 2$	$\geqq 4$

* Except for interpolation between the first two points in the table.

The above results are quite reasonable in view of the relatively large increment in X. Tests using smaller increments in X and uneven spacing of X were also satisfactory.

It was also discovered that for integration the following restrictions must be observed:

1. xlo ≦ xa (1).
2. xup ≧ xa (nop).

REMARK ON ALGORITHM 77
INTERPOLATION, DIFFERENTIATION, AND INTEGRATION [P. E. Hennion, *Comm. ACM*, Feb., 1962]

P. E. HENNION
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It was brought to my attention through the CERTIFICATION OF ALGORITHM 77 AVINT [V. E. Whittier, *Comm. ACM*, June, 1962] that restrictions on the upper and lower limits of integration existed, i.e., (1) $x10 \leqq xa$ (1), (2) $xup \geqq xa(nop)$. To remove these restrictions the following two changes should be made.

1. Before line *L*16: and after the statement *ib* := 2; place the following code:

```
      for ia := 1 step 1 until nop do begin
      if xa(ia) ≧ x10 then go to L17; ib := ib + 1; end;
L17:  ju 1 := nop + 1; for ia := 1 step 1 until nop do begin
      ju 1 := ju 1 − 1; if xa(ju 1) > xup end; ju 1 := ju 1 − 1;
```

2. Change line *L*13: to read:

```
L13:  if jm ≠ ib then go to L14;
```

REMARK ON ALGORITHM 77
INTERPOLATION, DIFFERENTIATION, AND INTEGRATION [P. E. Hennion, *Comm. ACM 5*, Feb. 1962]

P. E. HENNION
Giannini Controls Corp., Berwyn, Penn.

It was brought to my attention through the CERTIFICATION OF ALGORITHM 77 AVINT (V. E. Whittier, *Comm. ACM*, June, 1962) that restrictions on the upper and lower limits of integration existed, i.e., (1) $x1o \leqq xa(1)$, (2) $xup \geqq xa(nop)$. To remove these restrictions the following two changes should be made.

1. Replace the two lines starting at line *L*12: and ending after the statement *ib* := 2; with the following code:

```
L12:  sum := 0; syl := x1o; ib := 2, ju1 := nop;
      for ia := 1 step 1 until nop do begin
      if xa [ia] ≧ x1o then go to L17; ib := ib + 1; end;
L17:  for ia := 1 step 1 until nop do begin
      if xup ≧ xa [ju1] then go to L18; ju1 := ju1 − 1; end;
L18:  ju1 := ju1 − 1;
```

2. Change line *L*13: to read

```
L13:  if jm ≠ ib then go to L14;
```

ALGORITHM 78
RATIONAL ROOTS OF POLYNOMIALS WITH INTEGER COEFFICIENTS

C. PERRY
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```
comment This ALGOL procedure, named ratfact, for finding
  rational roots of polynomials with integer coefficients is a
  pedagogical example illustrating the use of the for statement
  described in section 4.6.3. Also, an extension suggested by
  J. Peck of the well-known polynomial evaluation by nesting,
  i.e. Horner's method, is used. The polynomial f(x)=a0 + a1x+
  ··· +anx^n with integer coefficients and with a0an≠o has a
  lowest term rational root p/q if and only if a0q^n + a1q^n-1p +
  ··· +an-1q p^n-1 + anp^n= 0, also q must be a factor of an and
  p a factor of a0 . Procedure RATFACT outputs the nonzero
  rational roots p/q by execution of the procedure whose formal
  name is print. The output procedure uses the string whose formal
  name is format for control of the output format;
procedure ratfact (a, n, print, format);
  integer array a[0:n]; integer n; procedure print; string
    format;
  begin integer i, p, q, r, t, f, g;
  p loop: for p := 1 step 1 until abs (a[0]) do
    begin comment if p is not a factor of a [0] or q is not a factor
      of a[n] then skip to the end of the loop for advance in the
      respective for list;
      if a[0] ≠ (a[0]÷p)×p then go to 1
      else q loop: for q := 1 step 1 until abs (a[n]) do
        begin if a[n] ≠ (a[n]÷ q)×q then go to 2
          else
          begin comment root test and print;
            comment start polynomial evaluation;
              f := g := a[0]; t := p;
              for i := 1 step 1 until n do
              begin r := a[i]×t;
                    f := f×q+r;
                    g := −g×q+r;
                    t := t×p;
              end polynomial evaluation;
              comment computing r saves one subscript
                evaluation;
            if f=0 then print (format, p, q);
            if g=0 then print (format,−p, q);
            comment print is the formal name of the procedure
              to be used to output the variables in the format
              specified by the string whose formal name is format;
          end root test and print;
      2: end q loop;
1: end p loop;
  end ratfact, without overflow test.
```

REMARK ON ALGORITHM 78
RATIONAL ROOTS OF POLYNOMIALS WITH INTEGER COEFFICIENTS [C. Perry, *Comm. ACM*, Feb. 1962]

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The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. It was noticed that a multiple rational root will only be printed once by the procedure.

CERTIFICATION OF ALGORITHM 78. RATFACT (C. Perry, *Comm. ACM 5*, Feb. 1962)

M. H. HALSTEAD
Navy Electronics Laboratory, San Diego, Calif.

RATFACT was copied in the Navy Electronics Laboratory International ALGOL Compiler, NELIAC, and tested on the UNIVAC M-490 Countess and the CDC 1604. Polynomials of order 2 through 6 were tested. No corrections were found necessary. It was noted that a polynomial whose coefficients included a common factor would produce superfluous values of p/q, in which this fraction was indeed a root, but one in which p and q contained a common factor.

ALGORITHM 79
DIFFERENCE EXPRESSION COEFFICIENTS

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```
procedure dicol (k, n, xp, xtab, coef);
value k, n; integer k, n; real xp;
array xtab, coef;
comment dicol produces the coefficients for the n ordinates
  (corresponding to the abscissae, xtab) in the n-point finite
  difference expression for the k-th derivative evaluated at xp.
  The method used is to determine the analytic expression for
  the k-th derivative of each coefficient in the n-point Lagrangian
  interpolation formula and evaluate it at xp. Note that k=0
  will produce the Lagrangian interpolation coefficients them-
  selves;
begin integer array xuse [1 : n-1]; real factk, sum, denom,
  part;
integer i, terms, j, m, high;
factk := 1.0; for i := 2 step 1 until k do factk := i×factk;
terms := n-k-1; if terms<0 then go to Z;
for j := 1 step 1 until n do
loop: begin sum := 0; denom := 1.0; part := 1.0;
      for i := 1 step 1 until n do
      if i ≠ j then denom := denom×(xtab [j] - xtab [i]);
      if terms = 0 then go to Y;
      m := 1; high := 1;
   A: if (high = j)∨(xtab [high] = xp) then
      A1: begin high := high + 1; go to A end A1;
      if high >.n then A2: begin m := m-1; if m>0
        then
      A3: begin high := xuse [m]+1; go to A end A3;
      go to X end A2;
      xuse [m] := high; m := m+1;
      if m≦terms then begin high := high + 1; go to
        A end;
      for i := 1 step 1 until terms do
        part := part×(xp - xtab [xuse [i]]);
      sum := sum + part; m := terms; part := 1.0;
      high := xuse [terms] + 1; go to A;
   Y: sum := 1.0;
   X: coef [j] := sum × factk/denom end loop;
     go to EXIT;
   Z: for i := 1 step 1 until n do coef [i] := 0;
   EXIT: end dicol
```

CERTIFICATION OF ALGORITHM 79
DIFFERENCE EXPRESSION COEFFICIENTS

[Thomas Giamo, *Comm. ACM*, Feb. 1962]

EVA S. CLARK
University of California at San Diego, La Jolla, California

The procedure was translated into FORTRAN and run on the CDC 1604. Reasonable accuracy was obtained for $k = 0, 4 \leqq n \leqq 12$. For increasing n and increasing k, the accuracy diminished. It was found that the execution time increased rapidly as n was increased. For $k = 0$, the following results were obtained:

n	*Approximate Number of Machine Operations*
4	1.3×10^3
6	6.9×10^3
8	3.8×10^4
10	1.8×10^5
12	8.6×10^5

The author indicated in a letter that the procedure was developed for use with small n and small k.

ALGORITHM 80
RECIPROCAL GAMMA FUNCTION OF REAL ARGUMENT
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```
real procedure RGR(x); real x; real procedure RGAM;
comment Procedure RGAM computes the real reciprocal
  Gamma function of real x for -1 < x < 1, utilizing Horner's
  method for polynomial evaluation of the approximation poly-
  nomial. RGR extends the range of RGAM by use of the formulae
  (1) 1/Gamma(x-1) = (x-1)/Gamma(x) for x<-1,
  (2) 1/Gamma(x+1) = 1/x×Gamma(x) for x<1.;
  begin real y;
        if x = 0.then begin RGR := 0; go to EXIT end
        if x = 1 then begin RGR := 1; go to EXIT end
        if x < 1 then go to BB;
        y := 1;
AA:     x := x - 1; y := y × x; if x > 1 then go to AA;
        if x = 1 then begin RGR := 1/y; go to EXIT end
        RGR := RGAM(x)/y; go to EXIT;
BB:     if x = -1 then begin RGR := 0; go to EXIT end
        if x > -1 then begin RGR := RGAM(x);
          go to EXIT end
        y := x;
CC:     x := x + 1; if x < -1 then begin y := y × x;
          go to CC end
        RGR := RGAM(x) × y;
EXIT:   end RGR;
real procedure RGAM(x); real x; integer i;
  real array B[0:13];
comment The algorithm for this routine was adapted from
  "University of Illinois Digital Computer, Auxiliary Library
  Routine B-17-328", by John Ehrman. Reference may also be
  made to Algorithm 34, dated February, 1961. Approximation
  accuracy is ±2^-35.;
begin real z;
  B[ 0] :=  1.00000 00000 00;  B[ 1] := -.42278 43350 92;
  B[ 2] := -.23309 37363 65;  B[ 3] := +.19109 11011 62;
  B[ 4] := -.02455 24908 87;  B[ 5] := -.01764 52421 18;
  B[ 6] := +.00802 32781 13;  B[ 7] := -.00080 43413 35;
  B[ 8] := -.00036 08514 96;  B[ 9] := +.00014 56243 24;
  B[10] := -.00001 75279 17;  B[11] := -.00000 26257.21;
  B[12] := +.00000 13285 54;  B[13] := -.00000 01812 20;
  z: = B[13];
  for i := 12 step -1 until 0 do z := z × x + B[i];
  RGAM := z × x × (x + 1)
end RGAM;
```

REMARKS ON:
ALGORITHM 34 [S14]
GAMMA FUNCTION
[M. F. Lipp, *Comm. ACM 4* (Feb. 1961), 106]
ALGORITHM 54 [S14]
GAMMA FUNCTION FOR RANGE 1 TO 2
[John R. Herndon, *Comm. ACM 4* (Apr. 1961), 180]
ALGORITHM 80 [S14]
RECIPROCAL GAMMA FUNCTION OF REAL ARGUMENT
[William Holsten, *Comm. ACM 5* (Mar. 1962), 166]
ALGORITHM 221 [S14]
GAMMA FUNCTION
[Walter Gautschi, *Comm. ACM 7* (Mar. 1964), 143]
ALGORITHM 291 [S14]
LOGARITHM OF GAMMA FUNCTION
[M. C. Pike and I. D. Hill, *Comm. ACM 9* (Sept. 1966), 684]

M. C. PIKE AND I. D. HILL (Recd. 12 Jan. 1966)
Medical Research Council's Statistical Research Unit,
University College Hospital Medical School,
London, England

Algorithms 34 and 54 both use the same Hastings approximation, accurate to about 7 decimal places. Of these two, Algorithm 54 is to be preferred on grounds of speed.

Algorithm 80 has the following errors:
(1) *RGAM* should be in the parameter list of *RGR*.
(2) The lines
if $x = 0$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x = 1$ **then begin** *RGR* := 1; **go to** *EXIT* **end**
should each be followed either by a semicolon or preferably by an **else**.
(3) The lines
if $x = 1$ **then begin** *RGR* := $1/y$; **go to** *EXIT* **end**
and
if $x < -1$ **then begin** $y := y \times x$; **go to** *CC* **end**
should each be followed by a semicolon.
(4) The lines
BB: **if** $x = -1$ **then begin** *RGR* := 0; **go to** *EXIT* **end**
and
if $x > -1$ **then begin** *RGR* := *RGAM*(x); **go to** *EXIT* **end**
should be separated either by **else** or by a semicolon and this second line needs terminating with a semicolon.
(5) The declarations of **integer** *i* and **real array** *B*[0:13] in *RGAM* are in the wrong place; they should come immediately after
begin real *z*;

With these modifications (and the replacement of the array *B* in *RGAM* by the obvious nested multiplication) Algorithm 80 ran successfully on the ICT Atlas computer with the ICT Atlas ALGOL compiler and gave answers correct to 10 significant digits.

Algorithms 80, 221 and 291 all work to an accuracy of about 10 decimal places and to evaluate the gamma function it is therefore on grounds of speed that a choice should be made between them. Algorithms 80 and 221 take virtually the same amount of computing time, being twice as fast as 291 at $x = 1$, but this advantage decreases steadily with increasing x so that at $x = 7$ the speeds are about equal and then from this point on 291 is faster—taking only about a third of the time at $x = 25$ and about a tenth of the time at $x = 78$. These timings include taking the exponential of *log-*

gamma.

For many applications a ratio of gamma functions is required (e.g. binomial coefficients, incomplete beta function ratio) and the use of algorithm 291 allows such a ratio to be calculated for much larger arguments without overflow difficulties.

ALGORITHM 81

ECONOMISING A SEQUENCE 1

BRIAN H. MAYOH

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```
procedure ECONOMISER 1 (desired property, costs, n, C);
  array costs; integer n;
    Boolean procedure desired property;
  Boolean array C;
begin comment Given a finite, monotonely increasing
  sequence of positive numbers, looked upon as prices, ECONO-
  MISER 1 selects the cheapest subsequence with a given prop-
  erty. The formal parameters are: Desired property, a function
  designator to answer the question: Does the subsequence held
  in array C possess the required property? n is (number of ele-
  ments in the sequence) + 1. Costs is an array of size [1:n].
  Costs[1] to costs[n-1] hold the numbers of the sequence and
  costs[n] is any arbitrary number greater than the sum of all
  other elements of costs. C is an array of the same size and indi-
  cates a subsequence by the rule: C[i] ≡ element i of the original
  sequence is in the subsequence. At exit from ECONOMISER 1,
  C indicates the cheapest subsequence. It is supposed that the
  original sequence has the desired property.;
  integer d, j, k, ℓ; real i;
  for j := 1 step 1 until n do C[j] := j = 1; d := 0;
  reenter: d := d+1;
  INSIDE: begin own real array prices [1:d];
            own Boolean array alternatives[1:d, 1:n];
            procedure ENTER SUCCESSORS;
            begin k := n-1;
              A: if ¬ C[k] then
                 begin k := k-1; go to A end; i := 0;
                 for j := 1 step 1 until n do
                 begin alternatives[ℓ,j]
                   := j ≠ k ∧ j ≠ k-1 ≡ C[j];
                   if alternatives[ℓ,j] then
                   i := i + costs[j]
                 end;
              B: k := k-1;
                 go to if k = 0 then find cheapest
                   else if C[k] then (if k=1 then
                     find cheapest else B)
                   else if k=1 then E
                     else if C[k-1] then D
                   else find cheapest;
              D: C[k-1] := false;
              E: C[k] := true; go to reenter
            end of ENTER SUCCESSORS;
            i := 0; for j := 1 step 1 until n do
            begin alternatives[d,j] := C[j]; if C[j] then
              i := i + costs[j]
            end; prices[d] := i;
          find cheapest: i := 0; for j := 1 step 1 until d do
            begin if prices[j] < i then
              begin ℓ := j; i := prices[ℓ] end
            end;
            for j := 1 step 1 until n do
            C[j] := alternatives[ℓ,j];
            if ¬ desired property then
              ENTER SUCCESSORS
          end of INSIDE;
end of ECONOMISER 1.
```

ALGORITHM 82

ECONOMISING A SEQUENCE 2

BRIAN H. MAYOH

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```
procedure ECONOMISER 2 (desired property, costs, n, C, r,
  Reject list); Boolean procedure desired property;
  integer n, r; array costs; Boolean array Reject list;
begin comment In some applications of ECONOMISER 1, it
  is simple to establish that some subsequences are redundant in
  the sense that any sequence containing them is certainly not
  the cheapest subsequence with the desired property. For such
  applications ECONOMISER 2 avoids all unnecessary calls of
  desired property. The new formal parameters are: r a variable
  whose value is initially 0 and is increased by 1 every time that
  desired property discovers a new redundant subsequence.
  Reject list an array of size [1:r,1:n]. Reject list [a,b] carries the
  answer to: Is element b of the original sequence in the a^th
  redundant subsequence found by desired property?;
  real i; integer d, j, k, ℓ; Boolean gapfilled, first time;
  procedure INSIDE (entrymaker); Boolean entrymaker;
  begin own real array prices[1:d];
        own Boolean array alternatives[1:d,1:n];
        procedure ENTER SUCCESSORS;
        begin integer c; Boolean array ssq[1:n];
            for j := 1 step 1 until n do ssq[j] := C[j];
            c := n−1;
        A:  if ¬ ssq[c] then begin c := c−1; go to A end;
            C[c] := false; C[c+1] := true;
            INSIDE (true);
            gapfilled := true;
        B:  c := c−1;
            go to if c=0 then F else if ssq[c] then
              (if c=1 then F else B) else if c=1 then
              E else if ssq[c−1] then D else F;
        D:  ssq[c−1] := false;
        E:  for j := 1 step 1 until n do C[j] := ssq[j] ≡ j≠c;
            INSIDE (true);
        F:  end of ENTER SUCCESSORS;
        if entrymaker then
        begin for j := 1 step 1 until r do
            begin for k := 1 step 1 until n do
              begin if ¬ C[k] ∧ Reject list[j,k] then
                go to G end;
              ENTER SUCCESSORS; go to H;
        G:  end;
            i := 0; if gapfilled then d := d+1;
            for j := 1 step 1 until n do
            begin alternatives[if gapfilled then
              d else ℓ, j] := C[j];
              if C[j] then i := i + costs[j]
            end; prices[if gapfilled then d else ℓ] := i
        end; if first time ∨ ¬ entrymaker then
        begin i := 0; gapfilled := first time := false;
          for j := 1 step 1 until d do
          begin if prices[j] < i then
            begin ℓ := j; i := prices[ℓ] end
          end;
            for j := 1 step 1 until n do
              C[j] := alternatives[ℓ,j];
            if desired property then go to found;
            ENTER SUCCESSORS; go to reenter
            end;
        H:  end of INSIDE;
        for j := 1 step 1 until n do C[j] := j=1;
        d := 0; first time := gapfilled := true;
reenter: INSIDE (first time);
found:
end of ECONOMISER 2;
```

ALGORITHM 83

OPTIMAL CLASSIFICATION OF OBJECTS

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```
procedure OPTIMUM COVERING FINDER (Pattern, population, set number, set prices, chosen sets, bounds, overflow);
  Boolean array Pattern, chosen sets; integer population, set number, bounds; array set prices; label overflow;
begin comment The number of objects in some given set is given by population. The procedure is given a classification of these objects by a collection of overlapping subsets. A cost is assigned to each subset. Then OPTIMUM COVERING FINDER selects the cheapest subcollection such that every object is contained in at least one of the subsets of the subcollection. set prices[i] carries the cost of subset i. Pattern is an array of size [1:set number,1:population] such that Pattern[a,b] = does subset a include object b. chosen sets[i] finally carries the answer to the question: Is set i in the cheapest subcollection? The programmer must restrict the amount of space available to the procedure by setting bounds. From experience bounds = set number ↑ 2 suffices to avoid most alarm exits to overflow.;
  Boolean array C[1:population], D[1:bounds, 1:population], R, S[1:bounds,1:set number];
  integer a, b, d, r, s;
  Boolean procedure HAVE WE A COVERING;
  begin procedure ADD to (Q,q,f); integer q;
        real f; Boolean array Q;
    begin if q=bounds then go to overflow else q := q+1;
      for a := 1 step 1 until set number do Q[q,a] := f
    end; for a := 1 step 1 until population do
          C[a] := false;
    for a := 1 step 1 until set number do
    begin if chosen sets[a] then
      for b := 1 step 1 until population do
      C[b] := C[b] ∨ Pattern[a,b]
    end; for a := 1 step 1 until population do
    begin if ¬ C[a] then go to E end;
    go to found;
E:  for d := 1 step 1 until s do
    begin for b := 1 step 1 until population do
      begin if C[b] ∧ ¬ D[d,b] then go to try another end;
      ADD to (R, r, chosen sets[a]);
      for b := 1 step 1 until set number do
      begin if chosen sets[b] ∧ ¬ S[d,b] then
        ADD to (R, r, S[d,a] ∨ a=b)
      end; go to F;
    try another:
    end of for statement labelled E;
    ADD to (S, s, chosen sets[a]);
    for a := 1 step 1 until population do D[s,a] := C[a];
F:  HAVE WE A COVERING := false
  end; r := s := 0;
  ECONOMISER 2 (HAVE WE A COVERING, set prices, set number, r, R, chosen sets);
found: end
```

ALGORITHM 84
SIMPSON'S INTEGRATION

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Astromechanics Research Division, Berwyn, Penn.

```
real procedure SIM (n, a, b, y);
value n, a, b; real a, b; integer n; array y;
comment This is a method for obtaining the approximate value
  of the definite integral of a continuous function when the in-
  tegral cannot be evaluated in elementary functions. Given
  y = f(x) and the ∫ₐᵇ y dx to be evaluated. Plot the curve f(x),
  and divide [a, b] evenly into n equal parts, erecting the ordi-
  nates y₀, y₁, ···, yₙ. Then the approximate value of the
  definite integral by Simpson's rule states that:
  ∫ₐᵇ f(x) dx = (b − a)/3n (y₀ + 4y₁ + 2y₂ + ··· + 4yₙ₋₁ + yₙ);
begin real s; integer i;
  s := (y[0] − y[n])/2;
  for i := 1 step 2 until n − 1 do s := s + 2 × y[i] + y[i+1];
  SIM := 2 × (b − a) × s/(3 × n)
end
```

CERTIFICATION OF ALGORITHM 84
SIMPSON'S INTEGRATION [P. E. Hennion, *Comm. ACM 5* (Apr. 1962)]

A. P. RELPH
The English Electric Co., Whetstone, England

Simpson's Integration was translated using the DEUCE ALGOL compiler and, with no corrections, gave satisfactory results.

It is not stated in the comment that integer n needs to be even.

REMARK ON ALGORITHM 84
SIMPSON'S INTEGRATION [Paul E. Hennion. *Comm. ACM*, Apr. 1962]

RICHARD GEORGE*
Particle Accelerator Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

In performing integration by the use of Simpson's rule, it is well known that the interval $[a, b]$ must be divided evenly into n equal parts, and that *it is essential for n to be an even number.*

In the published algorithm, there is neither a comment on this important restriction, nor a programmed test for the parity of n. It is therefore a potential trap for the unwary programmer.

CERTIFICATION OF ALGORITHM 84
SIMPSON'S INTEGRATION [P. E. Hennion, *Comm. ACM*, Apr. 62]

PETER G. BEHRENZ
Matematikmaskinnämnden, Stockholm, Sweden

SIM was successfully run on FACIT EDB using FACIT-ALGOL 1, which is a realization of ALGOL 60 for FACIT EDB. No changes in the program were necessary. To test SIM some polynomials were integrated.

ALGORITHM 85
JACOBI

THOMAS G. EVANS
Bolt, Beranek, and Newman*, Cambridge, Mass.

* This work has been sponsored by the Air Force Cambridge Research Laboratories, OAR (USAF), Detection Physics Laboratory, under contract AF 19(628)-227.

```
procedure JACOBI (A, S, n, rho);
value n, rho; integer n; real rho; real array A, S;
comment This procedure finds all eigenvalues and eigenvectors
  of a given square symmetric matrix by a modified Jacobi (iterative) method (cf. J. Greenstadt, "The determination of the characteristic roots of a matrix by the Jacobi method," in Mathematical Methods for Digital Computers, A. Ralston and H. S. Wilf, eds.). JACOBI is given a square symmetric matrix of order n stored in the array A. The initial contents of the array S are immaterial, as S is initialized by the procedure. At exit the k^th column of the array S contains the k^th of the n eigenvectors of the given matrix, and the diagonal element A[k, k] of the array A is the corresponing k^th eigenvalue. The parameter rho is the "accuracy requirement" introduced in the above reference, where a detailed flow chart of the method is given. The significance of rho is that the iteration terminates when, for every off-diagonal element A[i, j], abs (A[i, j]) < (rho/n) × norm1, where norm1 is a function only of the off-diagonal elements of the original matrix;
begin real norm1, norm2, thr, mu, omega, sint, cost, int1, v1,
  v2, v3;
  integer i, j, p, q, ind;
  comment Set array S = n × n identity matrix;
  for i := 1 step 1 until n do
  for j := 1 step 1 until i do
    if i = j then S[i, j] := 1.0
    else S[i, j] := S[j, i] := 0.0;
  comment Calculate initial norm (norm1), final norm (norm2),
  and threshold (thr);
  int1 := 0.0;
  for i :=2 step 1 until n do
    for j := step 1 until i−1 do
      int1 := int1 + 2.0 × A[i, j] ↑ 2;
  norm1 := sqrt (int1); norm2 := (rho/n) × norm1;
  thr := norm1; ind := 0;
main: thr := thr/n;
  comment The sweep through the off-diagonal elements begins here;
main1: for q := 2 step 1 until n do
       for p := 1 step 1 until q−1 do
         if abs (A[p, q]) ≧ thr then
         begin ind := 1; v1 := A[p, p]; v2 := A[p, q];
           v3 := A[q, q]; mu := 0.5 × (v1−v3);
           omega := (if mu = 0.0 then 1 else sign (mu)) ×
             (−v2)/sqrt(v2↑2 + mu↑2);
           sint := omega/sqrt(2.0 × (1.0 + sqrt(1.0 −
             omega↑2)));
           cost := sqrt (1.0 − sint↑2);
           for i := 1 step 1 until n do
           begin int1 := A[i, p] × cost − A[i, q] × sint;
             A[i, q] := A[i, p] × sint + A[i, q] × cost;
             A[i, p] := int1;
             int1 := S[i, p] × cost − S[i, q] × sint;
             S[i, q] := S[i, p] × sint + S[i, q] × cost;
             S[i, p] := int1
           end;
         for i := step 1 until n do
           begin A[p, i] := A[i, p]; A[q, i] := A[i q] end;
         A[p, p] := v1 × cost↑2 + v3 × sint↑2 − 2.0 ×
           v2 × sint × cost;
         A[q, q] := v1 × sint↑2 + v3 × cost↑2 + 2.0 ×
           v2 × sint × cost;
         A[p, q] := A[q, p] := (v1 − v3) × sint × cost +
           v2 × (cost↑2 − sint↑2)
       end;
  comment Now test to see if current tolerance exceeded and,
    if not, whether final tolerance reached;
  if ind = 1 then begin ind := 0; go to main1 end
  else if thr > norm2 then go to main
end JACOBI
```

CERTIFICATION OF ALGORITHM 85
JACOBI [T. G. Evans, *Comm. ACM*, Apr. 1962]

J. S. HILLMORE
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The statement

omega := (**if** *mu* = 0.0 **then** 1 **else** *sign* (*mu*)) × (−*V2*)/*sqrt*(*V2* ↑ 2+*mu* ↑ 2);

was changed to

omega := **if** *mu* = 0.0 **then** −1.0 **else** − *sign* (*mu*) × *V2*/*sqrt* (*V2* ↑ 2+*mu* ↑ 2);

When *mu* = 0, the original statement reduces to

omega := −*V2*/*sqrt* (*V2* ↑ 2);

and a truncation error in the evaluation of the square root can make the magnitude of omega slightly greater than unity. As a result, an error stop occurs during execution of the next statement when an attempt is made to evaluate *sqrt* (1 − *omega* ↑ 2).

In its modified form the algorithm has been successfully run using the Elliott ALGOL translator on the National-Elliott 803. Matrices of order up to fifteen have been solved, yielding eigenvalues and eigenvectors with an overall accuracy of seven decimal places.

CERTIFICATION OF ALGORITHM 85
JACOBI [Thomas G. Evans, *Comm. ACM* (Apr. 1962), 208]

P. NAUR
Regnecentralen, Copenhagen, Denmark

We have first run this algorithm in the GIER ALGOL system with the following corrections included:

1. The change given by J. S. Hillmore [*Comm. ACM 5* (Aug. 1962), 440] with capital *V* changed to *v*.

2. The 4th **for** clause corrected to read:

for j := 1 **step** 1 **until** $i - 1$ **do**

3. The last **for** clause corrected to read:

for i := 1 **step** 1 **until** n **do**

On closer examination we have found, however, that a significant number of superfluous operations could be eliminated in the innermost loop by rewriting the two **for** statements at the center of the algorithm as a single **for** statement, to read as follows:

```
. . . . .
cost := sqrt (1−sint ↑ 2);
for i := 1 step 1 until! n do
  begin if i ≠ p ∧ i ≠ q then
    begin int1 := A[i,p]; mu := A[i,q];
    A[q,i] := A[i,q] := int1 × sint + mu × cost;
    A[p,i] := A[i,p] := int1 × cost − mu + sint
    end;
  intl := S[i,p]; mu := S[i,q];
  S[i,q] := int1 × sint + mu × cost;
  S[i,p] := int1 × cost − mu × sint
  end;
A[p,p] := v1 × cost ↑ 2 + v3 × sint ↑ 2 − 2 × v2 × sint × cost;
. . . . .
```

This revision is particularly advantageous in systems having a comparatively slow subscript mechanism, such as GIER ALGOL, because it eliminates more than 3 out of 8 references to subscripted variables.

JACOBI has been tried with two different sets of matrices having known eigenvalues. In both cases a test program was set up to find the range of errors of the eigenvalues computed by JACOBI. In addition, the relations $Av - \lambda v = 0$ (A is the given matrix, v an eigenvector, and λ the corresponding eigenvalue) and $A - (ST)$ LAMBDA $S = 0$ (S is the matrix having the eigenvectors as columns and ST its transpose, and LAMBDA is the diagonal matrix of the eigenvalues) were used as checks. The test matrices were TESTMATRIX calculated by the revised algorithm 52 given in *Comm. ACM 6* (Jan. 1963), 39, and the following matrix suggested by Mr. H. B. Hansen:

HBH TESTMATRIX $[j,i]$ = HBH TESTMATRIX $[i,j]$
$= n + 1 - j \qquad j \geqq i$

having the eigenvalues $0.5/(1 - \cos((2\times i-1)\times pi/(2\times n+1)))$.

The results were as shown in Table 1 (GIER ALGOL works with floating numbers of 29 significant bits).

The compile time for the program which produced one of these tables was about 40 seconds. Run times were as follows:

Rho	n	*Original algorithm* TESTMATRIX ALG. 52 HBH TESTMATRIX (seconds)		*Revised algorithm* HBH TESTMATRIX (seconds)
$_{10}-3$	5			3
	10			22
	15			70
$_{10}-5$	5	3		5
	10	5	41	29
	15	13	148	99
$_{10}-8$	5	4	7	6
	6	5	12	
	7	5	18	
	8	5	25	
	10	13		38
	15	22		116

From these figures it looks as if TESTMATRIX, Algorithm 52, is atypical as far as solution by means of JACOBI is concerned. The much higher accuracy obtained for this matrix as compared with the HBH matrix points in the same direction.

For further comparison it may be mentioned that the algorithms published by J. H. Wilkinson [*Num. Math. 4* (1962), 354–376] also have been tested successfully with GIER ALGOL. Wilkinson's algorithms reduce the matrix to tridiagonal form by means of Householder's method and use Sturm sequences to find the eigenvalues and inverse iteration to find the eigenvectors. In GIER ALGOL this method is about 1.3 times as fast as JACOBI for the range of matrices considered here. JACOBI has the advantage that the eigenvectors are properly orthogonal, even in the case of multiple eigenvalues, and also has a much simpler logic. On the other hand if only some of the eigenvalues and/or eigenvectors are sought Wilkinson's algorithms will often offer much higher speed than JACOBI, which always finds them all.

TABLE 1
HBH TESTMATRIX

Range of true errors of eigenvalues					Range of deviations from relation Av − lambda v = 0						Range of deviations from relation A − (ST) LAMBDA S = 0					
Order	*j*	*error[j]*	*j*	*error[j]*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*
rho = $1.0_{10}-3$																
5	1	$-1.1_{10}-6$	3	$5.2_{10}-8$	1	1	$-1.7_{10}-4$	1	3	$2.0_{10}-4$	1	1	$-2.5_{10}-4$	5	5	$1.0_{10}-4$
10	9	$-7.9_{10}-5$	8	$3.5_{10}-5$	7	2	$-3.3_{10}-3$	6	6	$3.0_{10}-3$	1	1	$-4.2_{10}-3$	6	7	$3.2_{10}-3$
15	15	$-9.2_{10}-5$	12	$3.7_{10}-5$	6	3	$-1.7_{10}-3$	11	13	$1.7_{10}-3$	9	15	$-1.5_{10}-3$	8	9	$1.8_{10}-3$
rho = $1.0_{10}-5$																
5	1	$-1.1_{10}-6$	3	$6.0_{10}-8$	2	5	$-1.3_{10}-7$	5	2	$4.1_{10}-8$	1	2	$-1.6_{10}-7$	4	5	$4.5_{10}-8$
10	1	$-1.2_{10}-5$	2	$2.2_{10}-7$	7	3	$-2.7_{10}-5$	2	8	$2.2_{10}-5$	7	7	$-2.4_{10}-5$	2	8	$2.3_{10}-5$
15	1	$-3.5_{10}-5$	4	$3.9_{10}-7$	11	9	$-6.4_{10}-6$	7	2	$4.8_{10}-6$	11	12	$-5.3_{10}-6$	12	12	$4.7_{10}-6$
rho = $1.0_{10}-8$																
5	1	$-1.1_{10}-6$	3	$6.0_{10}-8$	2	5	$-1.3_{10}-7$	4	2	$6.5_{10}-9$	2	2	$-1.3_{10}-7$	4	4	$3.0_{10}-8$
10	1	$-1.2_{10}-5$	2	$2.2_{10}-7$	1	10	$-1.1_{10}-6$	4	2	$6.4_{10}-8$	1	2	$-5.7_{10}-7$	9	9	$8.2_{10}-8$
15	1	$-3.5_{10}-5$	4	$3.9_{10}-7$	1	14	$-3.4_{10}-6$	4	2	$3.9_{10}-7$	2	2	$-1.3_{10}-6$	15	15	$8.9_{10}-8$

TESTMATRIX, Algorithm 52

Range of true errors of eigenvalues					Range of deviations from relation Av − lambda v = 0						Range of deviations from relation A − (ST) LAMBDA S = 0					
Order	*j*	*error[j]*	*j*	*error[j]*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*	*Element*	*Vector*	*Error*
rho = $1.0_{10}-5$																
5	4	$-1.0_{10}-8$	1	.0	5	5	$-3.3_{10}-8$	5	4	$4.3_{10}-8$	5	5	$-5.1_{10}-8$	4	4	$3.9_{10}-8$
10	8	$-1.1_{10}-8$	4	.0	7	7	$-1.2_{10}-8$	9	6	$1.3_{10}-8$	7	8	$-5.1_{10}-9$	6	6	$2.0_{10}-8$
15	13	$-1.1_{10}-8$	6	.0	14	14	$-9.3_{10}-9$	10	10	$9.4_{10}-9$	8	9	$-1.9_{10}-9$	10	10	$1.3_{10}-8$
rho = $1.0_{10}-8$																
3	3	$-7.5_{10}-9$	1	$3.7_{10}-9$	3	1	$-2.8_{10}-9$	2	2	$9.3_{10}-9$	1	3	.0	1	2	$1.9_{10}-8$
4	4	$-5.6_{10}-9$	3	.0	2	2	$-4.5_{10}-9$	3	4	$3.3_{10}-9$	2	2	.0	2	3	$9.3_{10}-9$
5	4	$-1.0_{10}-8$	1	.0	5	4	$-4.9_{10}-9$	4	4	$5.8_{10}-9$	1	1	$-7.5_{10}-9$	3	4	$7.5_{10}-9$
6	4	$-4.7_{10}-9$	4	.0	4	3	$-2.8_{10}-9$	5	4	$3.6_{10}-9$	1	6	$-2.3_{10}-10$	4	5	$9.3_{10}-9$
7	4	$-5.1_{10}-9$	5	.0	6	6	$-2.8_{10}-9$	4	4	$3.4_{10}-9$	5	7	$-1.2_{10}-10$	5	6	$7.5_{10}-9$
8	7	$-7.5_{10}-9$	5	.0	5	5	$-6.0_{10}-9$	5	6	$3.2_{10}-9$	8	8	$-1.2_{10}-10$	7	7	$9.3_{10}-9$
9	6	$-4.4_{10}-9$	7	.0	6	5	$-5.1_{10}-9$	7	6	$3.2_{10}-9$	5	5	$-7.5_{10}-9$	8	8	$1.5_{10}-8$
10	8	$-1.5_{10}-8$	8	.0	8	9	$-9.3_{10}-9$	9	7	$7.2_{10}-9$	6	7	$-2.3_{10}-9$	9	9	$2.0_{10}-8$
11	10	$-7.5_{10}-9$	1	.0	9	10	$-6.5_{10}-9$	8	11	$3.0_{10}-9$	1	1	$-3.1_{10}-9$	8	8	$7.5_{10}-9$
12	8	$-5.0_{10}-9$	11	.0	10	6	$-7.6_{10}-9$	10	8	$2.4_{10}-9$	6	6	$-1.7_{10}-8$	4	4	$1.3_{10}-8$
13	12	$-1.1_{10}-8$	10	.0	10	11	$-6.9_{10}-9$	12	10	$9.1_{10}-9$	7	7	$-3.0_{10}-8$	12	12	$3.2_{10}-8$
14	10	$-1.5_{10}-8$	4	.0	13	13	$-1.1_{10}-8$	10	10	$6.7_{10}-9$	9	10	$-3.5_{10}-9$	6	6	$1.7_{10}-8$
15	13	$-1.1_{10}-8$	6	.0	14	14	$-1.1_{10}-8$	11	10	$3.5_{10}-9$	8	9	$-3.0_{10}-9$	6	11	$7.5_{10}-9$

ALGORITHM 86
PERMUTE
J. E. L. PECK AND G. F. SCHRACK
University of Alberta, Calgary, Alberta, Canada

```
procedure PERMUTE (x, n);
array x; integer n;
comment Each call of PERMUTE executes a permutation of
  the first n components of x. It assumes a nonlocal Boolean
  variable 'first', which when true causes the procedure to initial-
  ise the signature vector p. Thereafter 'first' remains false until
  after n! calls;
begin own integer array p[2:n]; integer i, k;
  if first then
  begin for i := 2 step 1 until n do
            p[i] := i; first := false
  end initialise;
  for k := 2 step 1 until n do
      begin integer km; real t;
        t := x[1]; km := k - 1;
        for i := 1 step 1 until km do
            x[i] := x[i+1];
        x[k] := t; p[k] := p[k] - 1;
        if p[k] ≠ 0 then go to EXIT;
        p[k] := k
      end k;
  first := true;
EXIT: end PERMUTE
```

CERTIFICATION OF ALGORITHM 86
PERMUTE [J. E. L. Peck and G. F. Schrock, *Comm. ACM*, Apr. 1962]
D. M. COLLISON
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. Values of n used were 0, 1, 2, 3, 4.

ALGORITHM 87
PERMUTATION GENERATOR

JOHN R. HOWELL
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```
procedure PERMUTATION (N, K);
value K, N; integer K; integer array N;
comment This procedure generates the next permutation in
  lexicographic order from a given permutation of the K marks
  0, 1, ···, (K−1) by the repeated addition of (K−1) radix K.
  The radix K arithmetic is simulated by the addition of 9 radix
  10 and a test to determine if the sum consists of only the original
  K digits. Before each entry into the procedure the K marks
  are assumed to have been previously specified either by input
  data or as the result of a previous entry. Upon each such entry a
  new permutation is stored in N[1] through N[K]. In case the
  given permutation is (K−1), (K−2), ···, 1, 0, then the next
  permutation is taken to be 0, 1, ···, (K − 1). A FORTRAN
  subroutine for the IBM 7090 has been written and tested for
  several examples;
begin integer i, j, carry;
  for i := 1 step 1 until K do
    if N[i] − K + i ≠ 0 then go to add;
  for i := 1 step 1 until K do N[i] := i − 1;
  go to exit;
add: N[K] := N[K] + 9;
    for i := 1 step 1 until K−1 do
      begin if K > 10 then go to B;
            carry := N[K−i+1]÷10; go to C;
        B:  carry := N[K−i+1]÷K;
        C:  if carry = 0 then go to test;
            N[K−i] := N[K−i] + carry;
            N[K−i+1] := N[K−i+1] −10 × carry
      end i;
test: for i := 1 step 1 until K do if N[i] − (K − 1) > 0
    then go to add;
    for i := 1 step 1 until K−1 do
      for j := i+1 step 1 until K do
        if N[i]−N[j] = 0 then go to add;
exit: end PERMUTATION GENERATOR
```

CERTIFICATION OF ALGORITHM 87
PERMUTATION GENERATOR [John R. Howell, *Comm. ACM*, Apr. 1962]

D. M. COLLISON
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The array N was removed from the value list in order that the permutations might be available outside the procedure. The algorithm was then run successfully with the Elliott ALGOL translator on the National-Elliott 803. It was rather slower than Algorithm 86.

CERTIFICATION OF ALGORITHM 87
PERMUTATION GENERATOR [John R. Howell, *Comm. ACM* (Apr. 1962)]

G. F. SCHRACK and M. SHIMRAT
University of Alberta, Calgary, Alb., Canada

PERMUTATION GENERATOR was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. The algorithm was timed for several small values of n. For purposes of comparison we include the times (in seconds) for PERMULEX (Algorithm 102).

n	3	4	5	6	7
PERMUTATION GENERATOR	3	41	558	—	—
PERMULEX	—	3	6	37	278

As can be seen from this table, PERMUTATION GENERATOR is considerably slower. It is probable that one could speed up PERMUTATION GENERATOR to a great extent by rearranging the algorithm in such a manner that the digits of a number to a certain base are permuted rather than the elements of a sequence.

REMARKS ON:

ALGORITHM 87 [G6]
PERMUTATION GENERATOR
[John R. Howell, *Comm. ACM 5* (Apr. 1962), 209]
ALGORITHM 102 [G6]
PERMUTATION IN LEXICOGRAPHICAL ORDER
[G. F. Schrak and M. Shimrat, *Comm. ACM 5* (June (1962), 346]
ALGORITHM 130 [G6]
PERMUTE
[Lt. B. C. Eaves, *Comm. ACM 5* (Nov. 1962), 551]
ALGORITHM 202 [G6]
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER
[Mok-Kong Shen, *Comm. ACM 6* (Sept. 1963), 517]

R. J. ORD-SMITH (Recd. 11 Nov. 1966, 28 Dec. 1966 and 17 Mar. 1967)
Computing Laboratory, University of Bradford, England

A comparison of the published algorithms which seek to generate successive permutations in lexicographic order shows that Algorithm 202 is the most efficient. Since, however, it is more than twice as slow as transposition Algorithm 115 [H. F. Trotter, Perm, *Comm. ACM 5* (Aug. 1962), 434], there appears to be room for improvement. Theoretically a "best" lexicographic algorithm should be about one and a half times slower than Algorithm 115. See Algorithm 308 [R. J. Ord-Smith, Generation of Permutations in Pseudo-Lexicographic Order, *Comm. ACM 10* (July 1967), 452] which is twice as fast as Algorithm 202.

ALGORITHM 87 is very slow.

ALGORITHM 102 shows a marked improvement.

ALGORITHM 130 does not appear to have been certified before. We find that, certainly for some forms of vector to be permuted, the algorithm can fail. The reason is as follows.

At execution of $A[f] := r$; on line prior to that labeled *schell*, f has not necessarily been assigned a value. f has a value if, and only if, the Boolean expression $B[k] > 0 \wedge B[k] < B[m]$ is **true** for at least one of the relevant values of k. In particular when matrix A is set up by $A[i] := i$; for each i the Boolean expression above is **false** on the first call.

ALGORITHM 202 is the best and fastest algorithm of the exicographic set so far published.

A collected comparison of these algorithms is given in Table I. t_n is the time for complete generation of $n!$ permutations. Times are scaled relative to t_8 for Algorithm 202, which is set at 100. Tests were made on an ICT 1905 computer. The actual time t_8 for Algorithm 202 on this machine *was* 100 seconds. r_n has the usual definition $r_n = t_n/(n \cdot t_{n-1})$.

TABLE I

Algorithm	t_6	t_7	t_8	r_6	r_7	r_8
87	118	—	—	—	—	—
102	2.1	15.5	135	1.03	1.08	1.1
130	—	—	—	—	—	—
202	1.7	12.4	100	1.00	1.00	1.00

ALGORITHM 88
EVALUATION OF ASYMPTOTIC EXPRESSION FOR THE FRESNEL SINE AND COSINE INTEGRALS

JOHN L. CUNDIFF
Engineering Experiment Station, Georgia Institute of Technology, Atlanta, Ga.

real procedure FRESNEL (u) Result: (frcos, frsin); **value** (u);

comment This procedure evaluates the Fresnel sine and cosine integrals for large u by expanding the anymptotic series given by

$$S(u) = \frac{1}{2} - \frac{\cos(x)}{\sqrt{2\pi x}}\left[1 - \frac{1\cdot 3}{(2x)^2} + \frac{1\cdot 3\cdot 5\cdot 7}{(2x)^4} - \cdots\right] - \frac{\sin(x)}{\sqrt{2\pi x}}\left[\frac{1}{2x} - \frac{1\cdot 3\cdot 5}{(2x)^3} + \frac{1\cdot 3\cdot 5\cdot 7\cdot 9}{(2x)^5} - \cdots\right]$$

and

$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}}\left[1 - \frac{1\cdot 3}{(2x)^2} + \frac{1\cdot 3\cdot 5\cdot 7}{(2x)^4} - \cdots\right] - \frac{\cos(x)}{\sqrt{2\pi x}}\left[\frac{1}{2x} - \frac{1\cdot 3\cdot 5}{(2x)^3} + \frac{1\cdot 3\cdot 5\cdot 7\cdot 9}{(2x)^5} - \cdots\right]$$

in which $x = \pi u^2/2$. Reference: PEARCEY, T. *Table of the Fresnel Integral to Six Decimal Places*. The Syndics of the Cambridge University Press, Melbourne, Australia (1956).;

```
begin   pi := 3.14159265; arg := pi × (u↑2)/2; temp := 1;
        argsq := 1/(4 × (arg↑2)); term := −3 × argsq;
        series := 1 + term; N := 3;
first:  if temp = series then go to second; temp := series;
        termi := term;
        term := −termi × (4 × N − 7) × (4×N − 5) × (argsq);
        if abs(term) > abs(termi) then go to second;
        series := temp + term; N := N + 1; go to first;
second: series2 := ½ × arg; temp := 0; term := series2;
        N := 2;
loop:   if series2 = temp then go to exit; termi := term;
        term := −termi × argsq × (4×N−5) × (4×N−3);
        if abs(term) > abs(termi) then go to exit;
        temp := series2; series2 := temp + term;
        N := N + 1; go to loop;
exit:   if u < 0 then half := −½ else half := ½;
        frcos := half + (sin(arg) × series − cos(arg) + series2)/
        (pi × u);
        frsin := half − (cos(arg) × series2 + sin(arg) × series)/
        (pi × u)
end FRESNEL;
```

REMARK ON ALGORITHMS 88, 89 AND 90
EVALUATION OF THE FRESNEL INTEGRALS

[J. L. Cundiff, *Comm. ACM*, May 1962]

MALCOLM D. GRAY
The Boeing Co., Seattle, Wash.

While coding these algorithms in FORTRAN for the IBM 7094, modifications were required (both in the formulation and in the language) before execution with any degree of speed and accuracy could be obtained. In the process it was found that the reference, *Pearcy*, contains an error in the formula for $C(u)$. This error is contained in Algorithm 88 in the formula

$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}}[\ ] - \cdots$$

The first minus sign above should be a plus sign.

After the necessary modifications were made, the three algorithms were found to be too large and uneconomical for our usage. A single algorithm, incorporating these three procedures, was written and is in current usage in a computer program which requires several thousand evaluations of each Fresnel integral.

ALGORITHM 89
EVALUATION OF THE FRESNEL SINE INTEGRAL

JOHN L. CUNDIFF
Engineering Experiment Station, Georgia Institute of Technology, Atlanta, Ga.

real procedure FRESNELSIN (u) Result: (frsin); **value** u;
comment This algorithm computes the Fresnel sine integral defined by,

$$S(u) = \int_0^u \sin \pi t^2/2 \, dt,$$

by evaluating the series expansion

$$S(x) = \sqrt{\frac{2x}{\pi}}\left[\frac{x}{3} - \frac{x^3}{7\cdot 3!} + \frac{x^5}{11\cdot 5!} - \frac{x^7}{15\cdot 7!} + \cdots\right]$$

where $x = \pi u^2/2$. Reference: PEARCEY, T. *Table of the Fresnel Integral to Six Decimal Places.* The Syndics of the Cambridge University Press, Melbourne, Australia (1956).;

```
begin  Pi2 := 1.5707963; x := Pi2 x (u↑2); frsin := x/3;
       frsqr := x↑2; N := 3; term := (−x × frsqr)/6;
       frsini := frsin + term/7;
Loop:  if frsin = frsini then go to exit; frsin := frsini;
       term := −term × frsqr/((2×N−1) × (2×N−2));
       frsini := frsin + term/(4×N−1); N := N + 1;
       go to Loop;
exit:  frsin := frsini × u
end FRESNELSIN;
```

REMARK ON ALGORITHMS 88, 89 AND 90
EVALUATION OF THE FRESNEL INTEGRALS

[J. L. Cundiff, *Comm. ACM*, May 1962]

MALCOLM D. GRAY
The Boeing Co., Seattle, Wash.

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$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}}[\ ] - \cdots.$$

The first minus sign above should be a plus sign.

After the necessary modifications were made, the three algorithms were found to be too large and uneconomical for our usage. A single algorithm, incorporating these three procedures, was written and is in current usage in a computer program which requires several thousand evaluations of each Fresnel integral.

ALGORITHM 90
EVALUATION OF THE FRESNEL COSINE INTEGRAL

JOHN L. CUNDIFF
Engineering Experiment Station, Georgia Institute of Technology, Atlanta, Ga.

real procedure FRESNELCOS (u) result: (frcos); **value** (u);
comment This algorithm computes the Fresnel cosine integral defined by

$$C(u) = \int_0^u \cos \frac{\pi t^2}{2}\, dt,$$

by evaluating the series expansion

$$C(u) = \sqrt{\frac{2x}{\pi}}\left[1 - \frac{x^2}{5\cdot 2!} + \frac{x^4}{9\cdot 4!} - \frac{x^6}{13\cdot 6!} + \cdots\right],$$

where $x = \pi u^2/2$. Reference: PEARCEY, T. *Table of the Fresnel Integral to Six Decimal Places*. The Syndics of the Cambridge University Press, Melbourne, Australia (1956).;

```
begin pi2 := 1.5707963; x := pi2 × (u↑2); frcos := 1;
      xsqr := x↑2; N := 3; term := −xsqr/2;
      frcoi := 1 + (term/5);
loop: if frcoi = frcos then go to exit; term := −term ×
      xsqr/((2×N−2 × (2×N−3)); frcos := frcoi; frcoi :=
      frcos + term/(4×N−3); N := N + 1; go to loop;
exits: frcos := u × frcos
end FRESNELCOS;
```

REMARK ON ALGORITHMS 88, 89 AND 90
EVALUATION OF THE FRESNEL INTEGRALS

[J. L. Cundiff, *Comm. ACM*, May 1962]

MALCOLM D. GRAY
The Boeing Co., Seattle, Wash.

While coding these algorithms in FORTRAN for the IBM 7094, modifications were required (both in the formulation and in the language) before execution with any degree of speed and accuracy could be obtained. In the process it was found that the reference, *Pearcy*, contains an error in the formula for $C(u)$. This error is contained in Algorithm 88 in the formula

$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}}[\ ] - \cdots.$$

The first minus sign above should be a plus sign.

After the necessary modifications were made, the three algorithms were found to be too large and uneconomical for our usage. A single algorithm, incorporating these three procedures, was written and is in current usage in a computer program which requires several thousand evaluations of each Fresnel integral.

ALGORITHM 91
CHEBYSHEV CURVE-FIT

ALBERT NEWHOUSE
University of Houston, Houston, Texas

```
procedure CHEBFIT(m, n, X, Y); integer m, n; array X, Y;
comment This procedure fits the tabular function Y(X) (given
  as m points (X, Y)) by a polynomial P = sum_{i=0}^{n} A_i X^i. This
  polynomial is the best polynomial approximation of Y(X) in
  the Chebyshev sense. Reference: STIEFEL, E. Numerical
  Methods of Tchebycheff Approximation, U. of Wisc. Press (1959),
  217-232;
begin array X[1:m], Y[1:m], T[1:m], A[0:n], AX[1:n+2],
    AY[1:n+2], AH[1:n+2], BY[1:n+2], BH[1:n+2];
  integer array IN [1:n+2]; real TMAX, H; integer i,
    j, k, imax;
  comment Initialize;
  k := (m-1)/(n+1);
  for 1 := 1 step 1 until n+1 do IN [i] := (i-1)×k + 1;
  IN[n+2] := m;
  START: comment Iteration begins;
  for i := 1 step 1 until n+2 do
    begin AX[i] := X[IN[i]];
          AY[i] := Y[IN[i]];
          AH[i] := (-1) ↑ (i-1)
    end i;
  DIFFERENCE: comment divided differences;
  for i := 2 step 1 until n+2 do
    begin
    for j := i-1 step 1 until n+2 do
    begin BY[j] := AY[j];
          BH[j] := AH[j]
    end j;
    for j := i step 1 until n+2 do
    begin AY[j] := (BY[j] -BY[j-1])/
            (AX[j] -AX[j-i+1]);
          AH[j] := (BH[j] -BH[j-1])/
            (AX[j] -AX[j-i+1])
    end j;
  end i;
  H := -AY[n+2]/AH[n+2];
  POLY: comment polynomial coefficients;
  for i := 0 step 1 until n do
    begin A[i] := AY[i] +AH[i] ×H;
          BY[i] := 0
    end i;
  BY[1] := 1; TMAX := abs(H); imax := IN[1];
  for i := 1 step 1 until n do
    begin
    for j := 0 step 1 until i-1 do
      begin
      BY[i+1-j] := BY[i+1-j] -BY[i-j] ×X[IN[i]];
      A[j] := A[j] +A[i] ×BY[i+1-j]
      end j;
    end i;
  ERROR: comment compute deviations;
  for i := 1 step 1 until m do
    begin T[i] := A[n];
      for j := 0 step 1 until n do T[i] := T[i] X[i] +A[n-j];
      T[i] := T[i] -Y[i];
      if abs(T[i]) ⩽ TMAX then go to L1;
      TMAX := abs(T[i]);
      imax := i
L1:   end i;
  for i := 1 step 1 until n+2 do
      begin
      if imax < IN[i] then go to L2;
      if imax = IN[i] then go to FIT end
      end i;
L2: if T[imax] × T[IN[i]] < 0 then go to L3;
  IN[i] := imax;
  go to START;
L3: if IN[1] < imax then go to L4;
  for i := 1 step 1 until n+1 do IN[n+3-i] := IN[n+2-i];
  IN[i] := imax;
  go to START;
L4: if IN[n+2] ⩽ imax then go to L5;
  IN[i-2] := imax;
  go to START;
L5: for i := 1 step 1 until n+1 do IN[i] := IN[i+1];
  IN[n+2] := imax;
  go to START;
FIT: end CHEBFIT
```

CERTIFICATION OF ALGORITHM 91
CHEBYSHEV CURVEFIT [A. Newhouse, *Comm. ACM*, May 1962]

ROBERT P. HALE
University of Adelaide, Adelaide, South Australia

The CHEBFIT algorithm was translated into FORTRAN and successfully run on an IBM 1620 when the following alterations were made:

(a) 2nd line after

```
                comment Initialize;
```

should read

```
  for i := 1 step 1 until n+1 do IN[i] := (i-1) × k + 1;
```

(b) 2nd and 3rd lines after

```
        Poly: comment polynomial coefficients;
```

should read

```
  begin A[i] := AY[i+1] + AH[i+1] × H;  BY[i+1] := 0
```

REMARKS ON ALGORITHM 91
CHEBYSHEV CURVE FIT [A. Newhouse, *Comm. ACM 5* (May 1962), 281; *6* (April 1963), 167]

PETER NAUR (Recd. 27 Sept. 1963)
Regnecentralen, Copenhagen, Denmark

In addition to the corrections noted by R. P. Hale [op. cit., April 1963] the following are necessary:

1. The arrays X, Y, and A cannot be declared to be local within the procedure body.
2. The identifier A must be included as a formal parameter.

3. It should be noted that the $X[i]$ must form a monotonic sequence.

4. **comment** cannot follow the colon following a label. This occurs in four places.

5. The **end** following **go to** *FIT* must be removed.

In addition, a large number of details can be made more concise and unnecessary operations can be eliminated. Also, it seems desirable to produce the maximum deviation as a result.

CERTIFICATION OF ALGORITHM 91 [E2] CHEBYSHEV CURVE-FIT [Albert Newhouse *Comm. ACM 5* (May 1962), 281; *6* (April 1963), 167; *7* (May 1964), 296]

J. BOOTHROYD (Recd. 15 May 1967 and 5 Sept. 1967)
University of Tasmania, Hobart, Tasmania, Australia.

In addition to the corrections noted by R. P. Hale [OP. CIT., April 1963] and P. Naur [OP. CIT., May 1964], the following changes are necessary:

1. The first statement should be $k := entier((m-1)/(n+1))$
2. A semi-colon should precede label *L*1.

With these changes the procedure ran successfully using Elliott 503 ALGOL.

Although this procedure is an implementation of a finite algorithm, roundoff errors may give rise to cyclic changes of the reference set causing the procedure to fail to terminate.

Algorithm 318 [J. Boothroyd, Chebyshev Curve-Fit(Revised), *Comm.ACM 10* (Dec. 1967), 801] avoids this cycling difficulty, uses less than half the auxiliary array space of Algorithm 91 and, on test, appears to be at least four times as fast.

ALGORITHM 92
SIMULTANEOUS SYSTEM OF EQUATIONS AND MATRIX INVERSION ROUTINE

DEREK JOHANN ROEK
Applied Physics Laboratory of Johns Hopkins University, Silver Spring, Maryland

```
procedure SIMULTANEOUS (U, W, C, X, B, n, kount, eps, absf) ;
array U, W, C, X, B ; integer n, kount ;
 real eps; real procedure absf;
comment This procedure solves the problem Ux := b for the vector x. It assumes the problem written in the form x'U' := b', where ' denotes transpose. The procedure is completed in n cycles and may be iterated kount times (kount ≦ 6). The transpose of U is in U[,] and the row vector b' is in B. The integer n is the dimension of U, and the solution row vector x' is in X. The matrix C is a check of accuracy. It should have b' in its first row, the first element b1 of b' along its main diagonal, and zeros elsewhere. The real number eps checks to see how close the actual result is to this theoretical one. Also if we let b' := (1, 0, ··· , 0), then this procedure finds the inverse W[,] of U. The function absf finds the absolute value of its argument. The procedure chooses the column vectors of U as the row vectors of W in the 0th cycle of the first iteration. For all subsequent iterations, the row vectors of W, computed at the nth cycle of the last iteration, are the row vectors of W in the 0th cycle ;
begin integer i, j, k, p ; real bh, b1, Z ;
 for j := 1 step 1 until n do
    for i := 1 step 1 until n do W[j, i] := U[i, j];
S1: for j := 1 step 1 until n do
      for i := 1 step 1 until n do C[i, j] := 0 ;
 for j := 1 step 1 until n do
    begin for k := 1 step 1 until n do
      begin C[j, j] := C[j, j] + W[j, k] × U[k, j] end;
      if j = 1 then Z := B[j]/C[j, j] else Z := 1/C[j, j];
      for k := 1 step 1 until n do
          begin X[k] := Z × W[j, k];
            W[j, k] := X[k]
          end k;
      for k := 1 step 1 until n do
          begin if k = j then go to S2 else
            for p := 1 step 1 until n do
                C[k, j] := C[k, j] + U[p, j] × W[k, p];
          if j = 1 then bh := B[j] else bh := 1;
          if k = 1 then b1 := B[j] else b1 := 0;
          for p := 1 step 1 until n do
          begin X[p] := bh × W[k, p] + (b1 − C[k, j]) × W[j, p];
            W[k, p] := X[p]
          end p;
S2:        if k = j ∧ j = n then go to S3
          end k;
    end j;
S3: for j := step 1 until n do
        if absf(absf(C[j, j]) − absf(B[1])) > eps then go to S4;
    go to S6;
S4: if kount > 0 then go to S5 else go to S6;
S5: kount := kount − 1;
    go to S1;
S6: for j := step 1 until n do
        X[j] := W[1, j];
S7: end SIMULTANEOUS
```

ALGORITHM 93
GENERAL ORDER ARITHMETIC

MILLARD H. PERSTEIN
Control Data Corp., Palo Alto, Calif.

```
procedure arithmetic (a, b, c, op);
integer a, b, c, op;
comment This procedure will perform different order arithmetic
  operations with b and c, putting the result in a. The order of the
  operation is given by op. For op = 1 addition is performed. For
  op = 2 multiplication, repeated addition, is done. Beyond these
  the operations are non-commutative. For op = 3 exponentiation,
  repeated multiplication, is done, raising b to the power c. Beyond
  these the question of grouping is important. The innermost
  implied parentheses are at the right. The hyper-exponent is
  always c. For op = 4 tetration, repeated exponentiation, is
  done. For op = 5, 6, 7, etc., the procedure performs pentation,
  hexation, heptation, etc., respectively.
    The routine was originally programmed in FORTRAN for the
  Control Data 160 desk-size computer. The original program
  was limited to tetration because subroutine recursiveness in
  Control Data 160 FORTRAN has been held down to four levels in
  the interests of economy.
    The input parameter, b, c, and op, must be positive integers,
  not zero;
begin own integer d, e, f, drop;
      if op = 1 then
      begin a := b + c;  go to 1
      end if op = 2 then d := 0;
      else d := 1;  e := c; drop := op - 1;
      for f := 1 step 1 until e do
      begin arithmetic (a, b, d, drop);
            d := a
      end;
1:    end arithmetic
```

CERTIFICATION OF ALGORITHM 93
GENERAL ORDER ARITHMETIC [Millard H. Perstein, *Comm. ACM* (June 1962)]

RICHARD GEORGE
Particle Accelerator Div. Argonne National Laboratory, Argonne, Ill.

Algorithm 93 was programmed for the IBM 1620, using "FORTRAN-recursion" (i.e., generous use of the copy rule). The program ran without any modifications and was tested through tetration. Further levels were available, but were too time-consuming to reach.

ALGORITHM 94
COMBINATION

JEROME KURTZBERG
Burroughs Corp., Burroughs Laboratories, Paoli, Pa.

```
procedure COMBINATION (J, N, K); value N, K; integer
  array J; integer N, K;
comment This procedure generates the next combination of N
  integers taken K at a time upon being given N, K and the pre-
  vious combination. The K integers in the vector J(1) ··· J(K)
  range in value from 0 to N − 1, and are always monotonically
  strictly increasing with respect to themselves in input and
  output format. If the vector J is set equal to zero, the first
  combination produced is N−K, ··· , N−1. That initial combina-
  tion is also produced after 0, 1, ··· , N−1, the last value in that
  cycle;
begin integer B, L;
      B := 1:
mainbody: if J(B)≧B then begin A := J(B) − B−1;
            for L := 1 step 1 until B do J(L) := L + A;
            go to exit end;
          if B = K then go to initiate;
          B := B + 1; go to mainbody;
initiate: for B := 1 step 1 until K do J(B) := N − K − 1 + B
exit:     end COMBINATION
```

CERTIFICATION OF ALGORITHM 94
COMBINATION [J. Kurtzberg, *Comm. ACM*, June 1962]

RONALD W. MAY
University of Alberta, Calgary, Alberta, Canada

Algorithm 94 was translated into FORTRAN for the IBM 1620 and run successfully with no corrections. The variable A, however, has not been declared.

CERTIFICATION OF ALGORITHM 94
COMBINATION [J. Kurtzburg, *Comm. ACM*, June, 1962]

R. E. GRENCH*
Reactor Eng. Div., Argonne National Laboratory, Argonne, Ill.

* Work supported by U. S. Atomic Energy Commission

Four changes were required in the algorithm.

1. The last sentence in the comment should read: That initial combination is also produced after 0, 1, ··· , $K-1$, the last value in that cycle;
2. The integer A was declared;
3. Parentheses were replaced by brackets in the subscript expressions;
4. A semicolon was inserted at the end of the initiate statement.

After the above changes were made the body of Algorithm 94 was tested on an LGP-30 computer using the Dartmouth College ALGOL-30 translator. The body tested satisfactorily and the time required to generate one J when $K = 5$ and $N = 15$ was 30 seconds.

Various tests should be included if this algorithm is to be used as a procedure. These tests might include a statement to check if $K > N$ and if the initial value of J is correct These two possibilities were investigated and it was found that improper J's are generated.

ALGORITHM 95

GENERATION OF PARTITIONS IN PART-COUNT FORM

FRANK STOCKMAL

System Development Corp., Santa Monica, Calif.

```
procedure partgen(c,N,K,G); integer N,K; integer array c;
  Boolean G;
comment This procedure operates on a given partition of the
  positive integer N into parts ≦ K, to produce a consequent
  partition if one exists. Each partition is represented by the
  integers c[1] thru c[K], where c[j] is the number of parts of the
  partition equal to the integer j. If entry is made with G = false,
  procedure ignores the input array c, sets G = true, and pro-
  duces the first partition of N ones. Upon each successive entry
  with G = true, a consequent partition is stored in c[1] thru c[K].
  For N = KX, the final partition is c[K] = X. For N = KX+r,
  1 ≦ r ≦ K−1, final partition is c[K] = X, c[r] = 1. When entry
  is made with array c = final partition, c is left unchanged and G
  is reset to false;
begin integer a,i,j;
        if ¬ G then go to first;
        j := 2;
        a := C[1];
test:   if a < j then go to B;
        c[j] := 1 + c[j];
        c[1] := a − j;
zero:   for i := 2 step 1 until j − 1
        do c[i] := 0;
        go to EXIT;
B:      if j = K then go to last;
        a := a + j × c[j];
        j := j + 1;
        go to test;
first:  G := true;
        c[1] := N;
        j := K + 1;
        go to zero;
last:   G := false;
EXIT: end partgen
```

ALGORITHM 96
ANCESTOR

ROBERT W. FLOYD
Armour Research Foundation, Chicago, Ill

```
procedure ancestor (m, n); value n; integer n; Boolean
  array m;
comment Initially m [i, j] is true if individual i is a parent of
  individual j. At completion, m [i, j] is true if individual i is an
  ancestor of individual j. That is, at completion m[i, j] is true
  if there are k, l, etc. such that initially m[i, k], m[k, l], ···, m[p, j]
  are all true. Reference: WARSHALL, S. A theorem on Boolean
  matrices, J.ACM 9(1962), 11-12;
begin
integer i, j, k;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
if m [j, i] then
for k := 1 step 1 until n do
if m [i, k] then
m [j, k] := true
end ancestor
```

CERTIFICATION OF ALGORITHM 96
ANCESTOR [Robert W. Floyd, *Comm. ACM*, June, 1962]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission

The body of this procedure was tested on the LGP-30 using the Dartmouth translator. After inclosing conditional statements in **begin end** brackets (apparently necessary for this translator), the procedure operated satisfactorily for the following matrices:

n=5, Time: 8′15″

FTTFF		FTTTT
FFFFT		FFFFT
FFFTF	→	FFFTT
FFFFT		FFFFT
FFFFF		FFFFF

n = 6, Time: 13′15″

FTTFFF		FTTTTT
FFFTFF		FFFTFT
FFFFTF	→	FFFTFT
FFFFFT		FFFFFT
FFFFFF		FFFFFF

n = 9, Time 31′2″

FTTFFFFFF		FTTTTTTTT
FFFFTFFFF		FFFFTTTTF
FFFTTFFFF		FFFTTTTTT
FFFFFFFFT		FFFFFTTTT
FFFFFTTFF	→	FFFFFTTTF
FFFFFFFTF		FFFFFFFTF
FFFFFFFTF		FFFFFFFTF
FFFFFFFFF		FFFFFFFFF
FFFFFTTFF		FFFFFTTTF

The correctness of these results was confirmed by inspection of the network diagrams.

ALGORITHM 97
SHORTEST PATH
ROBERT W. FLOYD
Armour Research Foundation, Chicago, Ill.

```
procedure shortest path (m, n); value n; integer n; array m;
comment Initially m[i, j] is the length of a direct link from
  point i of a network to point j. If no direct link exists, m [i, j] is
  initially 10↑10. At completion, m [i, j] is the length of the shortest
  path from i to j. If none exists, m [i, j] is 10↑10. Reference: WAR-
  SHALL, S. A theorem on Boolean matrices. J, ACM 9(1962), 11-12;
begin
integer i, j, k; real inf, s; inf := 10↑10;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
if m [j, i] < inf then
for k := 1 step 1 until n do
if m [i, k] < inf then
begin s := m [j, i] + m [i, k];
if s < m [j, k] then m [j, k] := s
end
end shortest path
```

ALGORITHM 98

EVALUATION OF DEFINITE COMPLEX LINE INTEGRALS

JOHN L. PFALTZ

Syracuse University Computing Center, Syracuse, N. Y.

```
procedure COMPLINEINTGRL(A, B, N, RSSUM);
  value A, B, N; real A, B, N; array RSSUM;
comment COMPLINEINTGRL approximates the complex line
  integral by evaluating the partial Riemann-Stieltjes sum
  ∑_{t=1}^{n} f(z_k)[z_t − z_{t−1}] where a ≦ t ≦ b and z_k ∈ (z_{t−1}, z_t). The
  programmer must provide 1) the procedures GAMMA(T, Z) to
  calculate z(t) on Γ, and FUNCT(Z, F) to calculate function
  values, and 2) the end points A and B of the parametric interval
  and N the number of subintervals into which [a, b] is to be
  partitioned;
begin integer I; real T, DELT; real array ZT, ZTL, DELZ,
      ZK, PART[1:2]; RSSUM[1] := 0.0; RSSUM[2] := 0.0;
      DELT := (B − A)/N; T := A;
line: GAMMA(T, ZT);
      if T = A then go to next;
      for I := 1 step 1 until 2 do
      begin
        DELZ[I] := ZT[I] − ZTL[I]; end;
      for I := 1 step 1 until 2 do
      begin
        ZK[I] := ZTL[I] + DELZ[I]/2.0; end;
      FUNCT(ZK, FZ);
      PART[1] := FZ[1] × DELZ[1] − FZ[2] × DELZ[2];
      PART[2] := FZ[1] × DELZ[2] + FZ[2] × DELZ[1];
      for I := 1 step 1 until 2 do
      begin
        RSSUM[I] := RSSUM[I] + PART[I]; end;
      if T < B − (0.25 × DELT) then go to next else go to
        exit;
next: for I := 1 step 1 until 2 do
      begin
        ZTL[I] := ZT[I]; end;
      T := T + DELT;
      go to line;
exit: end COMPLINEINTGRL.
```

ALGORITHM 99
EVALUATION OF JACOBI SYMBOL

STEPHEN J. GARLAND AND ANTHONY W. KNAPP
Dartmouth College, Hanover, N. H.

```
procedure Jacobi (n,m,r); value n,m;
integer n, m, r;
comment Jacobi computes the value of the Jacobi symbol (n/m),
  where m is odd, by the law of quadratic reciprocity. The param-
  eter r is assigned one of the values −1, 0, or 1 if m is odd. If m
  is even, the symbol is undefined and r is assigned the value 2.
  For odd m the routine provides a test of whether m and n are
  relatively prime. The value of r is 0 if and only if m and n have
  a nontrivial common factor. In the special case where m is prime,
  r = −1 if and only if n is a quadratic nonresidue of m;
begin
  integer s;
  Boolean p, q;
  Boolean procedure parity (x); value x; integer x;
    comment The value of the function parity is true if x is
      odd, false if x is even;
    begin
      parity := x ÷ 2 × 2 ≠ x
    end parity;
  if ¬ parity (m) then begin r := 2; go to exit end;
  p := true;
  loop: n := n − n ÷ m × m;
        q := false;
        if n ≦ 1 then go to done;
  even: if ¬ parity (n) then
        begin
          q := ¬ q;
          n := n ÷ 2;
          go to even
        end n now odd;
        if q then if parity ((m↑2 − 1)÷8) then p := ¬ p;
        if n = 1 then go to done;
        if parity ((m−1) × (n−1) ÷ 4) then p := ¬ p;
        s := m; m := n; n := s; go to loop;
  done: r := if n = 0 then 0 else if p then 1 else −1;
exit: end Jacobi
```

REMARK ON ALGORITHM 99
EVALUATION OF JACOBI SYMBOL [S. J. Garland and A. W. Knapp, *Comm. ACM 6*, June 1962]

RONALD W. MAY
University of Alberta, Calgary, Alberta, Canada

One syntactical error was found in this procedure. It occurs in the second **if** statement following the **label** even. The statement

```
if q then if parity ((m↑2−1)÷8) then
    p := ¬ p;
```

might be changed as follows.

```
if q then go to CHECK;
next 1: if n = 1 then go to done;
CHECK: if parity ((m ↑ 2 − 1) ÷ 8) then
    p := ¬ p;
go to next 1;
```

The two statements beginning with *CHECK* could be inserted before the **label** done and after the statement **go to** loop;.

ALGORITHM 100

ADD ITEM TO CHAIN-LINKED LIST

PHILIP J. KIVIAT

United States Steel Corp., Appl. Research Lab., Monroeville, Penn.

```
procedure inlist (t,info,m,list,n,first,flag,addr,listfull);
integer n,m,first,flag,t; integer array info,list,addr;
comment inlist adds the information pair {t,info} to the chain-
  link structured matrix list (i,j), where t is an order key ≧ 0, and
  info(k) an information vector associated with t. info(k) has di-
  mension m, list(i,j) has dimensions (n × (m+3)). flag denotes
  the head and tail of list(i,j), and first contains the address of the
  first (lowest order) entry in list(i,j). addr(k) is a vector con-
  taining the addresses of available (empty) rows in list(i,j).
  Initialization: list(i,m+2) = flag, for some i ≦ n. If list(i,j) is
  filled exit is to listfull;
begin integer i, j, link1, link2;
0: if addr [1] = 0; then go to listfull; i := 1;
1: if list [i,1] ≦ t
     then begin if list [i,2] ≠ 0 then begin link1 := m+2;
       link2 := m+3; go to 2 end; else begin if
       list [i,m+2] = flag then begin i := flag;
       link1 := m+3; link2 := m+2; go to 3 end;
       else begin i := i+1; go to 1 end end end;
     else begin link1 := m+3; link2 := m+2 end;
2: if list [i,link2] ≠ flag
     then begin k := i; i := list [i,link2];
       if (link2 = m+2 ∧ list [i,1] ≦ t) ∨
         (link2 ≠ m+2 ∧ list [i,1] > t) then go to 4;
       else go to 1 end;
     else begin list [i,link2] := addr [1] end;
3: j := addr [1]; list [j,link1] := i;
   list [j,link2] := flag; if link2 = m+2 then
   first := addr [1]; go to 5;
4: j := addr [1]; list [j,link1] := list [i,link1];
   list [i,link1] := list [k,link2] := addr [1];
   list [j,link2] := i;
5: list [j,1] := t; for i := 1 step 1 until m do
   list [j,i+1] := info [i]; for i := 1 step 1 until n−1 do
   addr [i] := addr [i+1]; addr [n] := 0
end inlist
```

ALGORITHM 101

REMOVE ITEM FROM CHAIN-LINKED LIST

PHILIP J. KIVIAT

United States Steel Corp., Appl. Res. Lab., Monroeville, Penn.

```
procedure outlist (vector,m,list,n,first,flag,addr);
integer n,m,first,flag; integer array vector,list,addr;
comment outlist removes the first entry (information pair with
  lowest order key) from list(i,j) and puts it in vector(k);
begin integer i;
for i := 1 step 1 until m+1 do vector[i] := list [first,i];
for i := n−1 step −1 until 1 do addr [i+1] := addr [i];
addr [1] := first;
if list [first,m+3] = flag then
  begin list [1,m+2] := flag; first := 1;
  for i := 1 step 1 until n do addr [i] := i end;
else begin first := list [first,m+3];
list [first,m+2] := flag end;
for i := 1 step 1 until m+3 do list [addr [1], i] := 0
end outlist
```

ALGORITHM 102
PERMUTATION IN LEXICOGRAPHICAL ORDER
G. F. SCHRACK AND M. SHIMRAT
University of Alberta, Calgary, Alberta, Canada

```
procedure PERMULEX(n,p);
integer n; integer array p;
comment Successive calls of the procedure will generate all
  permutations p of 1,2,3,···,n in lexicographical order. Before the
  first call, the non-local Boolean variable 'flag' must be set to
  true. If after an execution of PERMULEX 'flag' is false,
  additional calls will generate further permutations—if true, all
  permutations have been obtained;
begin integer array q[1:n]; integer i, k, t; Boolean flag2;
if flag then
  begin for i := 1 step 1 until n do
  p[i] := i; flag2 := true; flag := false;
  go to EXIT
  end initialize;
if flag2 then
  begin t := p[n]; p[n] := p[n−1]; p[n−1] := t;
  flag2 := false; go to EXIT
  end bypass;
flag2 := true; for i := n−2 step −1 until 1 do
  if p[i] < p[i+1] then go to A;
  flag := true; go to EXIT;
A: for k := 1 step 1 until n do q[k] := 0;
    for k := i step 1 until n do q[p[k]] := p[k];
    for k := p[i] + 1 step 1 until n do
    if q[k] ≠ 0 then go to B;
B: p[i] := k; q[k] := 0;
    for k := 1 step 1 until n do
    if q[k] ≠ 0 then begin i := i + 1; p[i] := q[k] end
    else if i ≧ n then go to EXIT;
EXIT:
end PERMULEX
```

REMARKS ON:

ALGORITHM 87 [G6]
PERMUTATION GENERATOR
[John R. Howell, *Comm. ACM 5* (Apr. 1962), 209]
ALGORITHM 102 [G6]
PERMUTATION IN LEXICOGRAPHICAL ORDER
[G. F. Schrak and M. Shimrat, *Comm. ACM 5* (June (1962), 346]
ALGORITHM 130 [G6]
PERMUTE
[Lt. B. C. Eaves, *Comm. ACM 5* (Nov. 1962), 551]
ALGORITHM 202 [G6]
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER
[Mok-Kong Shen, *Comm. ACM 6* (Sept. 1963), 517]

R. J. ORD-SMITH (Recd. 11 Nov. 1966, 28 Dec. 1966 and 17 Mar. 1967)
Computing Laboratory, University of Bradford, England

A comparison of the published algorithms which seek to generate successive permutations in lexicographic order shows that Algorithm 202 is the most efficient. Since, however, it is more than twice as slow as transposition Algorithm 115 [H. F. Trotter, Perm, *Comm. ACM 5* (Aug. 1962), 434], there appears to be room for improvement. Theoretically a "best" lexicographic algorithm should be about one and a half times slower than Algorithm 115. See Algorithm 308 [R. J. Ord-Smith, Generation of Permutations in Pseudo-Lexicographic Order, *Comm. ACM 10* (July 1967), 452] which is twice as fast as Algorithm 202.

ALGORITHM 87 is very slow.

ALGORITHM 102 shows a marked improvement.

ALGORITHM 130 does not appear to have been certified before. We find that, certainly for some forms of vector to be permuted, the algorithm can fail. The reason is as follows.

At execution of $A[f] := r$; on line prior to that labeled *schell*, f has not necessarily been assigned a value. f has a value if, and only if, the Boolean expression $B[k] > 0 \wedge B[k] < B[m]$ is **true** for at least one of the relevant values of k. In particular when matrix A is set up by $A[i] := i$; for each i the Boolean expression above is **false** on the first call.

ALGORITHM 202 is the best and fastest algorithm of the exicographic set so far published.

A collected comparison of these algorithms is given in Table I. t_n is the time for complete generation of $n!$ permutations. Times are scaled relative to t_8 for Algorithm 202, which is set at 100. Tests were made on an ICT 1905 computer. The actual time t_8 for Algorithm 202 on this machine *was* 100 seconds. r_n has the usual definition $r_n = t_n/(n \cdot t_{n-1})$.

TABLE I

Algorithm	t_6	t_7	t_8	r_6	r_7	r_8
87	118	—	—	—	—	—
102	2.1	15.5	135	1.03	1.08	1.1
130	—	—	—	—	—	—
202	1.7	12.4	100	1.00	1.00	1.00

ALGORITHM 103
SIMPSON'S RULE INTEGRATOR
GUY F. KUNCIR
UNIVAC Division, Sperry Rand Corp., San Diego, Calif.

```
procedure SIMPSON (a, b, f, I, i eps, N);
  value a, b, eps, N; integer N;
  real a, b, I, i, eps; real procedure f;
comment This procedure integrates the function f(x) using a
  modified Simpson's Rule quadrature formula. The quadrature is
  performed over j subintervals of [a,b] forming the total area I.
  Convergence in each subinterval of length (b−a)/2^n is indicated
  when the relative difference between successive three-point and
  five-point area approximations
      A3,j = (b−a)(g0 + 4g2 + g4)/(3·2^(n+1))
      A5,j = (b−a)(g0 + 4g1 + 2g2 + 4g3 + g4)/(3·2^(n+2))
  is less than or equal to an appropriate portion of the over-all
  tolerance eps (i.e., |(A5,j − A3,j)/A5,j | ≦ eps/2^n with n ≦ N).
  SIMPSON will reduce the size of each interval until this con-
  dition is satisfied.
    Complete integration over [a,b] is indicated by i = b. A value
  a ≦ i < b is indicates that the integration was terminated, leav-
  ing I the true area under f in [a,i]. Further integration over [i,b]
  will necessitate either the assignment of a larger N, a larger eps,
  or an integral substitution reducing the slope of the integrand in
  that interval. It is recommended that this procedure be used
  between known integrand maxima and minima.;
begin integer m, n; real d, h; array g[0:4], A[0:2], S[1:N, 1:3];
  I := i := m := n := 0;
  g[0] := f(a);
  g[2] := f((a + b)/2);
  g[4] := f(b);
  A[0] := (b − a) × (g[0] + 4 × g[2] + g[4])/2;
AA: d := 2↑n; h := (b − a)/4/d;
    g[1] := f(a + h × (4 × m + 1));
    g[3] := f(a + h × (4 × m + 3));
    A[1] := h × (g[0] + 4 × g[1] + g[2]);
    A[2] := h × (g[2] + 4 × g[3] + g[4]);
    if abs (((A[1] + A[2]) − A[0])/(A[1] + A[2])) > eps/d
      then begin m := 2 × m; n := n + 1;
             if n > N then go to CC;
             A[0] := A[1]; S[n,1] := A[2];
             S[n,2] := g[3]; S[n,3] := g[4];
             g[4] := g[2]; g[2] := g[1]; go to AA
           end
    else begin I := I + (A[1] + A[2])/3;
           m := m + 1; i := a + m × (b − a)/d;
BB:        if m = 2 × (m ÷ 2) then
             begin m := m ÷ 2; n := n − 1; go to BB end
         if (m ≠ 1) ∨ (n ≠ 0) then
           begin A[0] := S[n,1]; g[0] := g[4];
                 g[2] := S[n,2]; g[4] := S[n,3]; go to AA end
         end
CC: end SIMPSON
```

ALGORITHM 104
REDUCTION TO JACOBI
H. RUTISHAUSER
Eidg. Technische Hochschule, Zurich, Switzerland

```
procedure m21 (n, a, b, c, inform); value n;
  integer n; array a, b, c; procedure inform;
  comment: m21 transforms symmetric bandmatrix
```

$$\begin{pmatrix} a[1] & b[1] & c[1] & & & \\ b[1] & a[2] & b[2] & c[2] & & O \\ c[1] & b[2] & a[3] & b[3] & \ddots & \\ & c[2] & & \ddots & & c[n-2] \\ & & \ddots & & a[n-1] & b[n-1] \\ & O & & c[n-2] & b[n-1] & a[n] \end{pmatrix}$$

```
  represented by the arrays a, b, c by orthogonal transformation
  to Jacobi form which is represented by the arrays a, b. The
  method is described in H. RUTISHAUSER, "On Jacobi rotation
  patterns," to appear in Proc. Symposium in Experimental
  Arithmetic, Chicago, Apr. 12-14, 1962, Sect. 5. Note that decla-
  rations must be given for the arrays a, b, c with subscripts
  ranging from 1 to n. Also procedure inform must be declared.
  It may serve to use the Jacobi rotations occurring inside m21
  also for other purposes;
begin
  real p, g, d, s;
  integer k, j;
  b[n] := c[n] := c[n-1]: = 0;
  for k := 2 step 1 until n-1 do
  begin
    for j := k step 2 until n-1 do
    begin
      if k=j then
      begin
        p := sqrt(b[k-1]↑2 + c[k-1]↑2);
        if p=0 then go to ex;
        d := b[k-1]/p;
        s := -c[k-1]/p;
        b[k-1] := p;
        c[k-1] := 0
      end k=j
    else
      begin
        p := sqrt(c[j-2]↑2+g↑2);
        if p = 0 then go to ex;
        d := c[j-2]/p;
        s := -g/p;
        c[j-2] := p;
        p := d×b[j-1]-s×c[j-1];
        c[j-1] := s×b[j-1]+d×c[j-1];
        b[j-1] := p
      end j≠k;
common: g := 2×b[j]×d×s;
      p := a[j]×d×d-g+a[j+1]×s×s;
      b[j] := (a[j]-a[j+1])×d×s+b[j]×(d×d-s×s);
      a[j+1] := a[j]×s×s+g+a[j+1]×d×d;
      a[j] := p;
      p := d×c[j]-s×b[j+1];
      b[j+1] := s×c[j]+d×b[j+1];
      c[j] := p;
      g := -s×c[j+1];
      c[j+1] := d×c[j+1];
      inform (n, j, d, s);
      comment: The Jacobi rotation which has been performed
        in this turn of the j-loop is A := U^T A U with
```

$$U = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & O \\ & & d & s & & \\ & & -s & d & & \\ & O & & & 1 & \\ & & & & & 1 \end{pmatrix},$$

```
        where the d's and s's are located at the crosspoints of
        rows and columns j and j +1;
    end j;
ex: end k
end m21
```

ALGORITHM 105
NEWTON MAEHLY

F. L. BAUER AND J. STOER
Johannes Gutenberg-Universität, Mainz, Germany

```
procedure Newton Maehly (a, n, z, eps);
  value n, eps;
  array a, z;
  integer n;
  real eps;
  comment The procedure determines all zeros z[1:n] of the
    polynomial p(x) := a[0] × x↑n + ··· + a[n] of order n, if p(x)
    has only real zeros which have to be all different. The zeros
    z[i] are ordered according to their magnitude: z[1]>z[2]>
    ···>z[n]. The approximations for each zero will be improved
    by iteration as long as abs(x1−x0)>eps × abs(x1) holds
    for two successive approximations x0 and x1;
begin real aa, pp, qq, x0, x1;
  integer i, m, s;
  array b, p, q[0:n−1];
  procedure Horner(p, q, n, x, pp, qq);
    value n, x;
    array p, q;
    real pp, x, qq;
    integer n;
  begin real s, s1;
    integer i;
    s := s1 := 0;
    for i := 0 step 1 until n−1 do
    begin s := s×x+p[i];  s1 := s1×x+q[i];  end ;
    pp := s×x+p[n];  qq := s1;
    end;
    p[0] := aa := a[0];  x0 := pp := 0;  s := sign(a[0]);
    for i := 1 step 1 until n do
      if s × a[i]<0 then
        begin if pp=0 then pp := i;
              if x0<abs(a[i]) then x0 := abs(a[i]);
        end;
    x0 := if pp=0 then 0 else 1+exp(ln(abs(xo/aa))/pp);
  comment x0 is a first approximation for the largest zero which
    may be printed out at this point of the program;
  for i := 0 step 1 until n−1 do b[i] := (n−1)×a[i];
  for m := 1 step 1 uhtil n do
    begin
      iteration:
      Horner (a, b, n, x0, pp, qq);  x1 := x0−pp/qq;
      if abs(x1−x0)>eps×abs(x1) then
        begin x0 := x1;
          comment x0 is the last approximation for the zero
            being improved, which may be printed out at this
            point;
          go to iteration;
        end;
      z[m] := x1;
      comment z[m] := x1 is the mth zero of the polynomial;
      pp := b[0] := b[0] − aa;  q[0] := pp;
      if m<n then
        begin for i := 1 step 1 until n−1 do
                begin pp := p[i] := x1×p[i−1]+a(i);
                      pp := b[i] := b(i)−pp;
                      q[i] := x1×q[i−1]+pp;
                end;
              Horner (p, q, n−1, x1, pp, qq);
                x0 := x1−pp/qq;
              comment x0 is a first approximation for the
                next zero;
        end
    end
end Newton Maehly;
```

CERTIFICATION OF ALGORITHM 105
NEWTON MAEHLY [F. L. Bauer and J. Stoer, COMM. ACM, July 1962]

JOANNE KONDO
Burroughs Corp., Pasadena, Calif.

Algorithm 105 was successfully run on Burroughs 220 computer after the following correction had been made:

for i := 0 **step** 1 **until** $n-1$ **do** $b[i] := (n-1) \times a[i]$

changed to

for i := 0 **step** 1 **until** $n-1$ **do** $b[i] := (n-i) \times a[i]$.

The following polynomials were tested for real roots using this algorithm:

polynomial	*epsilon*	*accuracy*
(1) $x^3 - 2x^2 - 5x + 6$	0.0000001	10^{-8}
(2) $x^5 - 15x^4 + 85x^3 - 225x^2 + 274x - 120$	0.000001	10^{-6}

ALGORITHM 106
COMPLEX NUMBER TO A REAL POWER

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Computer Applications, Inc., San Diego, California

```
procedure POWC (x, y, w, A, B); value x, y, w;
  real x, y, w, A, B;
comment This procedure takes a complex number (x+iy) to
  a real power w. The result is A+iB=(x+iy)^w. This procedure
  must be used with caution because although it is formally cor-
  rect, it may not give the desired results. For example, if w is a
  reciprocal integer it does not follow that the desired power
  (a root) will be calculated;
begin real    THETA, PHI, R;
  if x>0 then begin THETA := 0.0;  go to SOL 1 end;
  if x<0∧y≧0 then begin THETA := 3.1415927;
    go to SOL 1 end;
  if x<0∧y<0 then begin THETA := 3.1415927;
    go to SOL 1 end;
  if x=0∧y=0 then begin A := B := 0.0;  go to RETURN end;
  if x=0∧y<0 then begin PHI := 1.5707963;  go to SOL 2 end;
  if x=0∧y>0 then begin PHI := −1.5707963;
    go to SOL 2 end;
  SOL 1: PHI := arctan (y/x)+THETA;
  SOL 2: R := sqrt (x×x+y×y);
         R := exp (w×ln(R));
         A := R×cos (w×PHI);
         B := R×sin (w×PHI);
  RETURN: end POWC
```

REMARK ON ALGORITHM 106
COMPLEX NUMBER TO A REAL POWER [Margaret L. Johnson and Ward Sangren, *Comm. ACM* 5, Jul. 1962]

GRANT W. ERWIN, JR.
The Boeing Co., Renton, Wash.

The comment "if W is a reciprocal integer it does not follow that the desired power (a root) will be calculated" might better read "if W is the reciprocal of an integer N, the procedure will calculate an nth root, but possibly not the particular nth root desired. E.g. $w = \frac{1}{3}, x = -1, y = 0$ uields $A = \frac{1}{2}, B = \frac{1}{2}\sqrt{3}$ rather than the simpler $A = -1, B = 0$."

The comment should be made that it is assumed that the arctan function yields a result between $-\pi/2$ and $\pi/2$.

The following four corrections should be made:

(1) **if** $x<0 \wedge y < 0$ **then begin** THETA: = 3.1415927;

should read:

··· THETA: = −3.1415927;

(2) **go to** RETURN **end**:

should read:

go to RETURN **end**;

(3) **if** $x = 0 \wedge y<0$ ···

should read:

if x = 0 ∧ y>0 ···

(4) **if** $x = 0 \wedge y > 0$

should read:

if $x = 0 \wedge y < 0$ ···

ALGORITHM 107
GAUSS'S METHOD

JAY W. COUNTS
University of Missouri, Columbia, Mo.

```
      procedure gauss (u, a, y);
      real array a, y; real temp; integer u;
      comment This procedure is for solving a system of
        linear equations by successive elimination of the un-
        knowns. The augmented matrix is a and u the number of
        unknowns. The solution vector is y. If the system hasn't
        any solution or many solutions, this is indicated by go
        to stop;
    begin
      integer i, j, k, m, n;
      n := 0;
ck0:  n := n+1;
      for k := n step 1 until u do if a[k, n]≠0 then go to ck1;
      go to stop;
ck1:  if k=n then go to ck2;
      for m := n step 1 until u+1 do
    begin
      temp := a[n, m]; a[n, m] := a[k, m]; a[k, m] := temp
    end;
ck2:  for j := u+1 step−1 until n do a[n, j] := a[n, j]/a[n, n];
      for i := k+1 step 1 until u do
      for j := n+1 step 1 until u+1 do
      a[i, j] := a[i, j]−a[i, n]×a[n, j];
      if n≠u then go to ck0;
      for i := u step−1 until 1 do
    begin
      y[i] := a[i, u+1]/a[i, i];
      for k := i−1 step−1 until 1 do
      a[k, u+1] := a[k, u+1]−a[k, i]×y[i]
    end end;
```

REMARK ON ALGORITHM 107
GAUSS'S METHOD [J. W. Counts, *Comm. ACM*, July 1962]

P. NAUR
Regnecentralen, Copenhagen, Denmark

Algorithm 107 cannot be recommended since it does not search for pivot and therefore will yield poor accuracy (cf. Remarks on Algorithm 42 above).

CORRECTION TO EARLIER REMARKS ON ALGORITHM 42 INVERT, ALG. 107 GAUSS'S METHOD, ALG. 120 INVERSION II, AND gjr [P. Naur, *Comm. ACM*, Jan. 1963, 38–40.]

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Regnecentralen, Copenhagen, Denmark

George Forsythe, Stanford University, in a private communication has informed me of two major weaknesses in my remarks on the above algorithms:

1) The computed inverses of rounded Hilbert matrices are compared with the exact inverses of unrounded Hilbert matrices, instead of with very accurate inverses of the rounded Hilbert matrices.

2) In criticizing matrix inversion procedures for not searching for pivot, the errors in inverting positive definite matrices cannot be used since pivot searching seems to make little difference with such matrices.

It is therefore clear that although the figures quoted in the earlier certification are correct as they stand, they do not substantiate the claims I have made for them.

To obtain a more valid criterion, without going into the considerable trouble of obtaining the very accurate inverses of the rounded Hilbert matrices, I have multiplied the calculated inverses by the original rounded matrices and compared the results with the unit matrix. The largest deviation was found as follows:

	Maximum deviation from elements of the unit matrix		
Order	*INVERSION II*	*gjr*	*Ratio*
2	$-1.49_{10}-8$	$-1.49_{10}-8$	1.0
3	$-4.77_{10}-7$	$-8.34_{10}-7$	0.57
4	$-9.54_{10}-6$	$-3.43_{10}-5$	0.28
5	$-7.32_{10}-4$	$-4.58_{10}-4$	1.6
6	$-1.61_{10}-2$	$-1.42_{10}-2$	1.1
7	$-5.78_{10}-1$	$-5.47_{10}-1$	1.1
8	$-1.20_{10}-2$	$-1.38_{10}1$	8.7
9	$-4.91_{10}1$	$-2.22_{10}1$	2.2

This criterion supports Forsythe's criticism. In fact, on the basis of this criterion no preference of INVERSION II or *gjr* can be made.

The calculations were made in the GIER ALGOL system, which has floating numbers of 29 significant bits.

ALGORITHM 108
DEFINITE EXPONENTIAL INTEGRALS A

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DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

```
real procedure As (n, b); value n, b; integer n; real b;
comment: This procedure computes a value of integral
  A_{n-1}(1, b) = ∫_1^∞ x^{n-1} exp(-bx) dx for any given positive integer, n,
  and any positive real parameter, b, by the recursion formula
  A_n(1, b) = A_0(1, b) + (n/b) A_{n-1}(1, b) with A_0(1, b) = exp(-b)/b;
begin integer m; real db; real array a[1:n];
        a[1] := exp (-b)/b;
      if n=1 then go to exit;
comment integral a[1] = A_0(1, b) was evaluated;
        db := 1/b; for m := 2 step 1 until n do a[m] :=
          a[1]+db×(m-1)×a[m-1];
comment integral a[n] = A_{n-1}(1, b) was evaluated;
        As := a[n] end As;
```

CERTIFICATION OF ALGORITHM 108
DEFINITE EXPONENTIAL INTEGRALS A [Yuri A. Kruglyak and Donald R. Whitman, *Comm. ACM 5* (July 1962)]

YURI A. KRUGLYAK
Kharkov State University, Kharkov, U.S.S.R. and
DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

Integrals $A_n(1,b)=\int_1^\infty x^n\exp(-bx)dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burrough's 220 computer using Burrough's Algebraic Compiler. The program was used to compute tables of $A_n(1,b)$ in the ranges $n=0(1)15$, and $b=0.01(0.01)30.14$. For example, for $n=0(1)15$, and $b=0.25$ and $b=24.0$, the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, 1959].

n	$b=0.25$	$b=0.25$ (Miller et al.)	$b=24.0$	$b=24.0$ (Miller et al.)
0	.31152031, 01	.31152031322856, 01	.15729727,−11	.15729727267830,−11
1	.15576015, 02	.15576015661428, 02	.16385132,−11	.16385132570656,−11
2	.12772332, 03	.12772332842371, 03	.17095154,−11	.17095154982051,−11
3	.15357951, 04	.15357951442168, 04	.17866621,−11	.17866621640586,−11
4	.24575835, 05	.24575837510601, 05	.18707497,−11	.18707497541261,−11
5	.49151976, 06	.49151986541516, 06	.19627122,−11	.19627122588926,−11
6	.11796476, 08	.11796479885167, 08	.20636507,−11	.20636507915061,−11
7	.33030132, 09	.33030143989988, 09	.21748707,−11	.21748708743056,−11
8	.10569642, 11	.10569646079911, 11	.22979295,−11	.22979296848848,−11
9	.38050711, 12	.38050725887992, 12	.24346962,−11	.24346963586148,−11
10	.15220284, 14	.15220290355200, 14	.25874294,−11	.25874295428724,−11
11	.66969248, 15	.66969277562880, 15	.27588778,−11	.27588779339328,−11
12	.32145238, 17	.32145253230182, 17	.29524115,−11	.29524116937494,−11
13	.16715523, 19	.16715531679695, 19	.31721955,−11	.31721957275639,−11
14	.93606928, 20	.93606977406291, 20	.34234200,−11	.34234202345285,−11
15	.56164156, 22	.56164186443775, 22	.37126102,−11	.37126103733633,−11

The accuracy is at least six significant figures over the entire range. This accuracy is completely satisfactory for all quantum chemical calculations.

ALGORITHM 109
DEFINITE EXPONENTIAL INTEGRALS B

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```
real procedure Bs(n, a); value n, a; integer n; real a;
comment This procedure computes a value of the integral
  B_{n-1}(a) = ∫_{-1}^{+1} x^{n-1} exp(-ax)dx for any given positive integer, n,
  and any real parameter, a. If |a|<alim an expansion of
  exp(-ax) is used, otherwise the recursion formula B_n(a) =
  [(-1)^n e^a - e^{-a} + nB_{n-1}(a)]/a with b_0(a) = 2 sinh(a)/a is used. The
  value of alim depends upon the highest n appearing in the
  calculations and upon the maximum errors in the last significant
  digits in the library procedures. For example, we have used
  alim=8 for n_max=16 with gamma=1×10^-8. The intrinsic func-
  tion mod(E1, E2) which requires two integer arguments, is the
  conventional modulus;
begin   integer m; real alim, delta, gamma, r, epsilon,
          s, k, a2, omega, da, jp, jm, q1, q2; real array
          b[1:n]; if a=0 then
L1:     begin if mod(n-1, 2)=0 then
L2:     begin b[n] := 2/n; go to exit end L2;
comment integral b[n] = B_{n-1}(0) for odd n was evaluated;
        b[n] := 0; go to exit end L1;
comment integral b[n] = B_{n-1}(0) for even n was evaluated;
        if abs(a) alim then
L3:     begin delta := gamma; if mod(n-1, 2)=0 then
L4:     begin r := 2/n; epsilon := r×delta; s := r;
          k := 0; a2 := a↑2;
Even:     k := k+2;
          r := r×a2×(n+k-2)/(k×(k-1)×(n+k));
          s := s+r; if r>epsilon then go to Even;
          b[n] := s+r;
        go to exit end L4;
comment integral b[n]=B_{n-1}(a) for odd n and |a|<alim was
          evaluated;
        r := 2×a/(n+1); omega := abs(r×delta);
          s := r; k := 1;
        a2 := a↑2;
Odd:    k := k+2;
          r := r×a2×(n+k-2)/(k×(k-1)×(n+k));
        s := s+r; if abs(r)>omega then go to Odd;
        b[n] := -(s+r); go to exit end L3;
comment integral b[n]=B_{n-1}(a) for even n and |a|<alim was
          evaluated;
        da := 1/a; jp := da×exp(a); jm := (da↑2)/jp;
          b[1] := jp-jm;
        if n=1 then go to exit;
comment integral b[1] = B_0(a) for |a|≧alim was evaluated;
        q1 := -1; q2 := 1; for m := 2 step 1 until n do
L5:     begin b[m] := q1×jp-jm+q2×da×b[m-1];
        q1 := -q1; q2 := q2+1 end L5;
comment integral b[n]=B_{n-1}(a) for integer n≧2 and |a|≧alim
          was evaluated;
exit:   Bs := b[n] end Bs;
```

CERTIFICATION OF ALGORITHM 109
DEFINITE EXPONENTIAL INTEGRALS B [Yuri A. Kruglyak, D. R. Whitman, *Comm. ACM 5* (July 1962)]

YURI A. KRUGLYAK
Kharkov State University, Kharkov, U.S.S.R., and
DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

Integrals $B_n(a) = \int_{-1}^{+1} x^n \exp(-ax)dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burroughs-220 computer using a Burroughs Algebraic Compiler. The program was used to compute tables of $B_n(a)$ in the ranges $n=0(1)15$, and $a=0.00(0.01)32.54$. For example, for $n=0(1)15$ and $a=0.25$, and $a=24.0$ the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, Austin, 1959].

n	$a=0.25$	$a=0.25$ (Miller et al.)	$a=24.0$	$a=24.0$ (Miller et al.)
0	.20208984, 01	.20208985344653, 01	.11037134, 10	.110371342208, 10
1	-.16771064, 00	-.16771066117520, 00	-.10577253, 10	-.105772536282, 10
2	.67921322, 00	.67921324506375, 00	.10155696, 10	.101556964184, 10
3	-.10074584, 00	-.10074585827159, 00	-.97676725, 09	-.976767216847, 09
4	.40896479, 00	.40896480211998, 00	.94091887, 09	.940918885936, 09
5	-.72008754,-01	-.72008756636929,-01	-.90768866, 09	-.907688654174, 09
6	.29268836, 00	.29268837517905, 00	.87679129, 09	.876921258533, 09
7	-.56030292,-01	-.56030294023170,-01	-.84798262, 09	-.847982638338, 09
8	.22792911, 00	.22792912573392, 00	.82105258, 09	.821052542631, 09
9	-.45856272,-01	-.45856272975462,-01	-.79581870, 09	-.795818718590, 09
10	.18664760, 00	.18664761544688, 00	.77212229, 09	.772122289331, 09
11	-.38809718,-01	-.38809719373731,-01	-.74982404, 09	-.749824039467, 09
12	.15803198, 00	.15803200452627, 00	.72880141, 09	.728801402343, 09
13	-.33640562,-01	-.33640563670387,-01	-.70894600, 09	-.708945995807, 09
14	.13702696, 00	.13702696892367, 00	.69016158, 09	.690161591189, 09
15	-.29686662,-01	-.29686663616401,-01	-.67236245, 09	-.672362427583, 09

The accuracy is at least six significant figures in the ranges mentioned above. This accuracy is enough for the majority of quantum chemistry calculations.

ALGORITHM 110
QUANTUM MECHANICAL INTEGRALS OF SLATER-TYPE ORBITALS

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```
real procedure INTSOLI (n, r, za, ab, As, Bs) Result:
  (s, i1, i2, i3); value n, r, za, zb; integer n; real r, za, zb;
  real array a[1:8], b[1:8], G[1:2×n]; integer array bc[1:2×n,
  1:2×n]; real procedure As, Bs;
comment Procedure INTSOLI computes the quantum mechan-
  ical integrals  s=⟨ψ^ai_n00 | ψ^bi_210⟩          (overlap integral),
                 i1=⟨ψ^ai_n00 | Z_a*/r_ai | ψ^bi_210⟩  (exchange integral),
                 i2=⟨ψ^ai_n00 | Z_b*/r_bi | ψ^ai_n00⟩  (coulomb integral),
  and            i3=⟨ψ^bi_210 | Z_a*/r_ai | ψ^bi_210⟩  (coulomb integral).
  Here | ψ^ai_nlm⟩ is a Slater-type orbital of electron i centered on
  atomic nucleus a. The integer n is the effective principal quan-
  tum number with values 1, 2, 3 and 4. Z_a*=za and Z_b*=zb
  are effective nuclear charges. r_bi is the distance of electron
  i from nucleus b. The input parameter r is the distance be-
  tween the two centers a and b. All physical quantities are
  given in atomic units;
begin   integer q, t, c, m;
          real g, zsa, zsb, ks, p, pt, lilya, s, k1, exc, i1, pppt,
          k2, sue, i2, pmpt, ptmp, k3, i3;
          bc[1, 1] := bc[2, 1] := bc[2, 2] := 1;
        for q := 3 step 1 until 2×n do
L6:     begin bc[g, 1] := 1; for t := 2 step 1 until g−1 do
          bc[q, t] := bc[q−1, t−1]+bc[q−1, t];
          bc[q, q] := 1 end L6;
comment binomial coefficients bc[q, t]=C(q−1, t−1) were computed
          using the recursion formula C(q, t)=C(q−1, t−1)+C(q−1, t);
procedure As(n, b) Result: (a[n]); value n, b; integer n;
          real b;
comment procedure As computes a value of integral A_{n−1}(1, b)
          [see Algorithm 108, "Definite Exponential Integrals A," by Yuri A. Kruglyak and D. R. Whitman,
          Comm. ACM (July 1962)]. Any identifier occurring
          within the As is specified to be local to the As;
begin   integer m; real db; a[1] := exp(−b)/b;
          if n=1 then go to exitAs; db := 1/b;
          for m := 2 step 1 until n do a[m] := a[1] +
          db×(m−1)×a[m−1]
exitAs: end As;
procedure Bs(n, a) Result: (b[n]); value n, a; integer n;
          real a;
comment procedure Bs computes a value of integral B_{n−1}(a)
          [see Algorithm 109, "Definite Exponential Integrals B" by Yuri A. Kruglyak and D. R. Whitman,
          Comm. ACM (July 1962)]. Any identifier occurring
          within the Bs is specified to be local to the Bs;
begin   integer m; real alim, delta, gamma, r, epsilon,
          s, k, a2, omega, da, up, jm, q1, q2;
          if a=0 then begin if mod(n−1, 2)=0
          then begin b[n] := 2/n; go to exitBs end;
          b[n] := 0; go to exitBs end;
          if abs(a)<alim then begin delta := gamma;
comment we have used alim=8 and gamma=1×10^−8;
          if mod(n−1, 2)=0 then begin r := 2/n;
          epsilon := r×delta;
          s := r; k := 0; a2 := a↑2;
Even:     k := k+2;
          r := r×a2×(n+k−2)/((k×(k−1)×(n+k));
          s := s+r; if r>epsilon then go to Even;
          b[n] := s+r;
          go to exitBs end; r := 2×a/(n+1);
          omega := abs(r×delta);
          s := r; k := 1; a2 := a↑2;
Odd:      k := k+2;
          r := r×a2×(n+k−2)/(k×(k−1)×(n+k));
          s := s+r; if abs(r)>omega then go to Odd;
          b[n] := −(s+r); go to exitBs end; da := 1/a;
          jp := da×exp(a);
          jm := (da↑2)/jp; b[1] := jp−jm;
          if n=1 then go to exitBs;
          q1 := −1; q2 := 1; for m := 2 step 1 until n
          do begin b[m] := q1×jp−jm+q2×da×b[m−1];
          q1 := −q1; q2 := q2+1 end
exitBs:   end Bs;
          g := 1; for m := 1 step 1 until 2×n do g := g/m;
          G[2×n] := g;
comment 1/(2n)!=G[2×n] was evaluated;
          zsa := za/n; zsb := zb/2; ks := (r/2)↑(n+3)×
          (2×zsa)↑(n+1/2)×zsb↑(5/2)×G[2×n]↑(1/2);
          p := r×(zsa+zsb)/2;
          pt := r×(zsa−zsb)/2;
          for c := 1 step 1 until n+3 do
ABSI:     begin As(c, p) Result: (a[c]);
          Bs(c, pt) Result: (b[c])
          end ABSI;
S:        lilya := 0; for m := 0 step 1 until n do lilya :=
          lilya+bc[n+1, m+1]×(a[n−m+2]×(b[m+1]+
          b[m+3])−b[m+2]×(a[n−m+1]+a[n−m+3]));
          s := ks×lilya;
I1:       k1 := ks×2×za/r; exc := 0;
          for m := 0 step 1 until n−1 do
          exc := exc+bc[n, m+1]×(a[n−m+1]×(b[m+1]+
          b[m+3])−b[m+2]×(a[n−m]+a[n−m+2]));
          i1 := k1×exc;
I2:       pppt := p+pt; k2 := (r/2)↑(2×n)×(2×zsa)↑
          (2×n+1)×zsb×G[2×n];
          for c := 1 step 1 until 2×n do
BA2:      begin As(c, pppt) Result: (a[c]);
          Bs(c, pppt) Result: (b[c])
          end BA2; sue := 0;
          for m := 0 step 1 until 2×n−1 do
          sue := sue+bc[2×n, m+1]×a[2×n−m]×b[m+1];
          i2 := k2×sue;
I3:       pmpt := p−pt; ptmp := −pmpt;
          k3 := (r/2)↑4×2×za×zsb↑5;
          for c := 1 step 1 until 4 do
AB3:      begin As(c, pmpt) Result: (a[c]);
          Bs(c, ptmp) Result: (b[c])
          end AB3; i3 := k3×(a[2]×(b[1]+2×b[3])−b[2]×
          (a[1]+2×a[3])+a[4]×b[3]−a[3]×b[4]) end
          INTSOLI;
```

CERTIFICATION OF ALGORITHM 110 QUANTUM MECHANICAL INTEGRALS OF SLATER-TYPE ORBITALS [Yuri A. Kruglyak and Donald R. Whitman, *Comm. ACM 5* (July 1962)]

YURI A. KRUGLYAK
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DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

This procedure was written and tested in the Burroughs 220 version of the ALGOL language in the spring of 1961 at Case Institute of Technology. The program was used to compute tables of quatnum mechanical integrals s, $i1$, $i2$, and $i3$ in the ranges: r(Å)=0.64(0.02)1.40(0.10)3.10; Z_b*=0.25(0.50)3.75, 3.90, 4.25, 4.55, 4.75, 5.20, 5.25; Z_a*=0.7, 1.0 for n=1; 1.3(1.0)3.3 for n=2; 0.2, 2.2(1.0)4.2 for n=3; and 0.2, 2.2, 3.2 for n=4. The table at the right shows typical results compared with values from *Integraltafeln zur Quantenchemie* by H. Preuss (Springer-Verlag, 1957), Zweiter Band. Accuracy is at least six significant figures in the ranges mentioned above. This is ample for the overwhelming majority of quantum chemistry calculations.

Certification of INTSOLI

Input				*K. and W. Result*		*Preuss' Result*		
n	*r*	*za*	*zb*			Notation		Table No.
1	5	0.5	0.2	*s*	0.14841691	0.5 0.1 [1a 3b]	0.148417	23
1	1	4.5	8.0	*s*	0.35203437	4.5 4.0 [1a 3b]	0.352034	30
2	1	20	20	*s*	0.25032133×10^{-1}	10 10 [2a 3b]	0.250321×10^{-1}	40
1	5	0.5	0.2	*i*1	0.22058816	0.5 0.1 $5[a^{-1} \mid$ 1a 3b]	0.220588	59
1	1	4.5	8.0	*i*1	0.96587055	4.5 4.0 $1[a^{-1} \mid$ 1a 3b]	0.965871	66
2	1	20	20	*i*1	0.58102500×10^{-1}	10 10 $1[a^{-1} \mid$ 2a 3b]	0.581025×10^{-1}	76
1	1	0.5	0.2	*i*2	0.44818080	0.5 0.5 $1[b^{-1} \mid$ 1a 1a]	0.448181	41
1	5	0.5	0.2	*i*2	0.97641725	0.5 0.5 $5[b^{-1} \mid$ 1a 1a]	0.976417	45
2	1	20	20	*i*2	0.99999530	10 10 $1[b^{-1} \mid$ 2a 2a]	0.100000×10^{1}	58
1	1	10	1	*i*3	0.26217432	0.5 0.5 $1[b^{-1} \mid$ 3a 3a]	0.262174	41
1	1	10	10	*i*3	0.11093011×10^{1}	5 5 $1[b^{-1} \mid$ 3a 3a]	0.110929×10^{1}	50
1	1	10	20	*i*3	0.10300137×10^{1}	10 10 $1[b^{-1} \mid$ 3a 3a]	0.103001×10^{1}	58

ALGORITHM 111

MOLECULAR-ORBITAL CALCULATION OF MOLECULAR INTERACTIONS

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DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

```
real procedure SOLI(n, za, zb, rem, coef2, r1, E1, dr1, drk1,
  acc, acc1, rk2, rk1, dr2, asy, rk3, dr3, As, Bs, RESULT) Result:
  (ra, Ep, Em, ca, ca2, cb, cb2, DEa, DEb, s, i1, i2, i3, haa, hab,
  hbb); value n, za, zb, rem, coef2, r1, E1, dr1, rk1, drk1, acc,
  acc1, rk2, dr2, asy, rk3, dr3; integer n, rem; real otherwise;
  real array a[1:8], b[1:8], G[1:8], zsap [1:9], rp[1:8], ans[1:rem];
  real procedure As, Bs, RESULT;
comment This procedure calculates a one-electron approximation to the energy of interaction of molecular species by the use of the molecular-orbital (MO) method with a linear combination of Slater-type orbitals (LCSTO). The wave function used is |φ⟩=c_a |ψ^a_n00⟩+c_b |ψ^b_210⟩, where |ψ^a_n1m⟩ is a STO centered on nucleus a. The effective principal quantum number n takes the integral value 1, 2, 3 or 4. The Hamiltonian used is: ℋ_ab = −Δ/2−Z_a*/r_a−Z_b*/r_b+Z_a*Z_b*/R_ab. Here Z_a* and Z_b* are effective nuclear charges, r_a and r_b the distances of the electron from nucleus a and b, and R_ab is the distance between nuclei a and b. The calculations are in atomic units, while the output ra is in Angstroms and DEa and DEb are in kcal/gm-ion. Abbreviations of the following type are used: Za = Z_a*, ra = R_ab(Å), haa = ⟨ψ^a_n00 | ℋ_ab | ψ^a_n00⟩, DEa = D(a, b+electron), e1 = ⟨ψ^a_n00 | −Δ/2−Z_a*/ra | ψ^a_n00⟩. The values of coef1 and coef2 are 627.71 (kcal/gm-ion) and 0.5291Å, respectively. r1, E1, dr1, dr2, dr3, acc, acc1, and asy are control parameters. The accuracy of the calculations (acc, acc1) is 1×10^−5. The initial values of R_ab and E_ are conveniently: r1=0.4(Å), and E1=100(a.u.). The steps are: dr1=0.1, dr2=0.4, and dr3=0.01, all in Angstroms. asy is −1×10^−3 (a.u.);
begin
  integer q, t, c, m, f; real otherwise;
procedure As(n, b) Result: (a[n]); value n, b; integer n;
    real b;
  comment any identifier occurring within the As is specified
    to be local to the As;
  begin integer m; real db; a[1] := exp(−b)/b;
    if n=1 then go to exitAs; db := 1/b;
    for m := 2 step 1 until n do a[m] := a[1]+db×
      (m−1)×a[m−1]
  exitAs: end As;
procedure Bs(n, a) Result: (b[n]); value n, a; integer n;
    real a;
  comment any identifier occurring within the Bs is specified
    to be local to the Bs;
  begin integer m; real otherwise; if a=0 then begin if
    mod(n−1, 2)=0 then begin b[n] := 2/n;
    go to exitBs end; b[n] := 0; go to exitBs end;
    if abs(a)<alim then begin delta := gamma;
    if mod(n−1, 2)=0 then begin r := 2/n;
    epsilon := r×delta; s := r; k := 0; a2 := a↑2;
  Even: k := k+2; r := r×a2×(n+k−2)/(k(k−1)(n+k));
    s := s+r; if r>epsilon then go to Even;
    b[n] := s+r; go to exitBs end;
    r := 2×a/(n+1); omega := abs(r×delta);
    s := r; k:=1; a2 := a↑2;
  Odd: k := k+2; r := r×a2×(n+k−2)/(k(k−1)(n+k));
    s := s+r; if abs(r)>omega then go to Odd;
    b[n] := −(s+r); go to exitBs
  end; da := 1/a; jp := da×exp(a);
    jm := (da↑2)/jp; b[1] := jp−jm;
  if n=1 then go to exitBs; q1 := −1; q2 := 1;
    for m := 2 step 1
  until n do begin b[m] := q1×jp−jm+
    q2×da×b[m−1];
  q1 := −q1; q2 := q2+1 end
  exitBs: end Bs;
procedure Result(coef1); real coef1;
comment RESULT computes Ep, Em, ca, ca2, cb, cb2, DEa, DEb, s, i1, i2, i3, nn, haa, hab, hbb. Important: RESULT and any identifier occurring within the RESULT enter SOLI as nonlocal entities;
begin r := ra×br; rp[1] := r; for c := 2 step 1 until
    n+4 do rp[c] := rp[c−1]×rp[1]; p := r×sum;
    pt := r×dif; ks := rp[n+3]×zss;
    for c:= 1 step 1 until n+3 do begin As(c, p)
    Result: (a[c]); Bs(c, pt) Result: (b[c]) end;
    lilya := 0; for m := 0 step 1 until n do lilya :=
    lilya+bc[n+1, m+1]×(a[n−m+2]×
    (b[m+1]+b[m+3])−b[m+2]×(a[n−m+1]
    +a[n−m+3])); s := ks×lilya: 1i12 := 2×s;
    k1 := ks×za/r; exc := 0; for m := 0 step 1
    until n−1 do exc := exc+bc[n, m+1]×(a[n−
    m+1]×(b[m+1]+b[m+3])−b[m+2]×(a[n−m]+
    a[n−m+2])); i1 := k1×exc; pppt := p+pt;
    k2 := rp[2×n]×zsbd; for c := 1 step 1 until
    2×n do begin As(c, pppt) Result: (a[c]);
    Bs(c, pppt) Result: (b[c]) end; sue := 0;
    for m := 0 step 1 until 2×n−1 do sue :=
    sue+bc[2×n, m+1]×a[2×n−m]×b[m+1];
    i2 := k2×sue; pmpt := p−pt;
    ptmp := −pmpt; k3 := rp[4]×z5;
    for c := 1 step 1 until 4 do begin As(c, pmpt)
    Result: (a[c]); Bs(c, ptmp) Result: (b[c]) end;
    i3 := k3×(a[2]×(b[1]+2×b[3])−b[2]×(a[1]+2×
    a[3])+a[4]×b[3]−a[3]×b[4]);
comment Two-center integrals s, i1, i2, and i3 were computed [see Algorithm 110, "Quantum Mechanical Integrals of Slater-Type Orbitals," by Yuri A. Kruglyak and D. R. Whitman, Comm. ACM (July 1962)]; nn := zz/(2×r); e2pnn := e2+nn;
  haa := e1−e2+nn; hbb := e2pnn−i3; hab := e2pnn×s−i1;
  den := 2−s×1i12; bsr := haa+hbb−hab×1i12;
  root := sqrt(bsr↑2−2×den×(haa×hbb−hab↑2));
  Ep := (bsr+root)/den; Em := (bsr−root)/den;
  ans[f] := Em; DEa := coef1×(e2−Em);
  DEb := coef1×(e1−Em); Emhaa := Em−haa;
  Emhbb := Em−hbb; ES := Em×s; habmES := hab−ES;
  caDcb1 := habmES/Emhaa; cbDca2 := habmES/Emhbb;
  if abs(Emhaa)>abs(Emhbb) then begin col := caDcb1↑2;
  cb2 := 1/(1+1i12×caDcb1+col); ca2 := cb2×col;
  ca := sqrt(ca2); cb := ca/caDcb1 go to NATA end;
  co2 := cbDca2↑2; ca2 := 1/(1+1i12×cbDca2+co2);
  cb2 := ca2×co2; ca := sqrt(ca2); cb := ca×cbDca2
NATA: end RESULT;
Begin of program: bc[1, 1] := bc[2, 1] := bc[2, 2] := 1;
  for q := 3 step 1 until 8 do begin bc[q, 1] := 1; for t := 2
```

```
    step 1 until q−1 do bc[q, t] := bc[q−1, t−1]+bc[q−1, t];
    bc[q, q] := 1 end;
IZM:  g := 1; for m := 1 step 1 until 2×n do g := g/m;
      G [2×n]:=g; zsa := za/n; zsap[1] := zsa×2;
      for c := 2 step 1
      until 2×n+1 do xsap[c] := zsap[c−1]×zsap[1];
      D := zsap[2×n+1]×G[2×n]; DS := sqrt(D);
      e1 := −zsap[2]×0.125×(4×n−3)/(2×n−1);
      zsb := zb×0.5; sum := zsa+zsb; dif := zsa−zsb;
      zsb5 := zsb↑5; zss := DS×sqrt(zsb5);
      zsbd := zsb×D; z5 := 2×za×zsb5; zz := za×zb;
      e2 := −(zsb↑2)/2; br := 0.5/coef2; f := 1;
      ans[1] := E1; ra := r1;
KOM:  ra := ra+dr1; if ra>rk1 then ra := ra+drk1;
      f := f+1; RESULT (coef1); if ans [f]−ans[f−1]≦
      acc then begin if ra>rk2 then go to IZM;
      go to KOM end; ansf := ans[f]; d1 := ra;
CLEV: ra := ra+dr2; RESULT (coef1); if e1<e2 then
      begin if Em−e1≦asy∧ra<rk3 then go to CLEV;
      go to KHAR end; if e1≧e2 then begin if Em−e2≦
      asy∧ra<rk3 then go to CLEV; go to KHAR end;
KHAR: ra := d1; ans[f−1] := ansf;
CASE: ra := ra−dr3; f := f+1; RESULT (coef1);
      if ans[f]−ans[f−1]≦acc1 then go to CASE;
      go to IZM end SOLI;
```

ALGORITHM 112
POSITION OF POINT RELATIVE TO POLYGON

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```
Boolean procedure POINT IN POLYGON (n, x, y, x0, y0);
value n, x0, y0; integer n; array x, y; real x0, y0;
comment if the points (x[i], y[i]) (i = 1, 2, ··· , n) are—in
  this cyclic order—the vertices of a simple closed polygon and
  (x0, y0) is a point not on any side of the polygon, then the pro-
  cedure determines, by setting "point in polygon" to true,
  whether (x0, y0) lies in the interior of the polygon;
begin integer i; Boolean b;
  x[n + 1] := x[1]; y[n + 1] := y[1]; b := true;
  for i := 1 step 1 until n do
    if (y < y[i] ≡ y > y[i + 1]) ∧
      x0 − x[i] − (y0 − y[i]) × (x[i + 1] − x[i])/(y[i + 1] − y[i]) <0
    then b := ¬ b;
  POINT IN POLYGON := ¬ b;
end POINT IN POLYGON
```

CERTIFICATION OF ALGORITHM 112
POSITION OF POINT RELATIVE TO POLYGON

[M. Shimrat, *Comm. ACM*, Aug. 1962]

RICHARD HACKER
The Boeing Co., Seattle Wash.

The Boolean procedure *POINT IN POLYGON* was programmed in FORTRAN for the IBM 7090. The algorithm gave satisfactory results except for a case such as the following:

Let the polygon points be: (0, 0), (1, 0), (2, 1), (1, 2), (0, 2).

In this case the procedure would not detect that the point (1, 1) is in the polygon. However, the correct result was obtained by changing:

```
if (y<y[i] ≡ y > y[i+1])∧
```

to read:

```
if (y0≦y[i] ≡ y0 > y[i+1])∧
```

ALGORITHM 113
TREESORT
ROBERT W. FLOYD
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```
procedure TREESORT (UNSORTED, n, SORTED, k); value
  n, k;
integer n, k; array UNSORTED, SORTED;
comment TREESORT sorts the smallest k elements of the n-
  component array UNSORTED into the k-component array
  SORTED (the two arrays may be the same). The number of
  operations is on the order of 2 × n + k × log2(n). The number
  of auxiliary storage cells required is on the order of 2 × n. It is
  assumed that procedures are available for finding the minimum
  of two quantities, for packing one real number and one integer
  into a word, and for obtaining the left and right half of a packed
  word. The value of infinity is assumed to be larger than that of
  any element of UNSORTED;
begin integer i, j; array m[1:2 × n − 1];
for i := 1 step 1 until n do m[n + i − 1] := pack (UNSORTED
  [i], n + i − 1);
for i := n − 1 step − 1 until 1 do m[i] := minimum (m[2 × i],
  m[2 × i + 1]);
for j := 1 step 1 until k do
  begin SORTED [j] := left half (m[1]); i := right half (m[1]);
    m[i] := infinity;
  for i := i ÷ 2 while i > 0 do m[i] := minimum (m[2 × i], m[2 ×
    i + 1])
  end
end TREESORT
```

ALGORITHM 114

GENERATION OF PARTITIONS WITH CONSTRAINTS

FRANK STOCKMAL

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```
procedure CP GENERATOR (N, K, H, p, F, Z); integer
  N, K, H; integer array p; Boolean F, Z;
comment CP GENERATOR generates a partition of N into K
  parts, no part greater than H. Each partition is represented by
  the array of parts p[1] thru p[K], where p[1] ≧ p[2] ≧ ··· ≧ p[K].
  Initial entry is made with F = true and Z = true if parts = 0
  are allowable, or F = true and Z = false if only nonzero parts
  are desired. Upon initial entry, procedure ignores the input
  array p, sets F = false, and generates the initial partition.
  Subsequent calls made with F = false will cause
  procedure to operate upon the input partition to produce
  another partition if one exists, so that all possible unpermuted
  partitions with the specified constraints will be produced if CP
  GENERATOR is allowed to operate upon its previous output.
  When this scheme is followed, and initial entry is made with
  F = true, Z = true, K = N, H = N, all possible un-
  permuted partitions of N will be produced. Upon generating
  the last partition, procedure resets F to true. The input param-
  eters are restricted as follows: K ≧ 1, H ≧ 1, p[1] ≧ p[2]
  ≧ ··· ≧ p[K]. For Z = true, N is restricted to the range
  0 ≦ N ≦ KH, and for Z = false, K ≦ N ≦ KH. A call should
  not be made with p[1] − p[K] < 2 and F = false;
begin integer a, b, i, j, q, r;
  if F then go to first;
  a := p[1] − p[2] − 2; j := 2;
test: if p[1] − p[j] ≧ 2 then go to divide;
  a := a − 1 + j × (p[j] − p[j + 1]); j := j + 1; go to test;
first: if Z then go to alpha;
  a := N − K; p[K] := 0; go to beta;
alpha: a := N; p[K] := −1;
beta: F := false; j := K;
divide: b := H − 1 − p[j]; q := entier (a/b); r := a − b × q;
  for i := 1 step 1 until q do p[i] := H;
  if q = K then go to last;
  for i := q + 1 step 1 until j do p[i] := 1 + p[j];
  p[q + 1] := r + p[q + 1];
  if p[1] − p[K] ≧ 2 then go to exit;
last: F := true;
exit: end CP GENERATOR
```

ALGORITHM 115
PERM

H. F. TROTTER
Princeton University, Princeton, N. J.

```
procedure PERM (x, n); value n;
integer n; array x;
comment This algorithm was inspired by the procedure
  PERMUTE of Peck and Schrack (Algorithm 86, Comm. ACM
  Apr. 1962) and performs the same function. Each call of PERM
  changes the order of the first n components of x, and n! succes-
  sive calls will generate all n! permutations. A nonlocal Boolean
  variable 'first' is assumed, which must be true when PERM is
  first called, to cause proper initialization. The first call of PERM
  makes 'first' false, and it remains so (unless changed by the
  external program) until the exit from the (n!)th call of PERM.
  At that time x is restored to its original order and 'first' is made
  true.
    The excuse for adding PERM to the growing pile of permuta-
  tion generators is that, at the expense of some extra own storage,
  it cuts the manipulation of x to the theoretical minimum of n!
  transpositions, and appears to offer an advantage in speed. It
  also has the (probably useless) property that the permutations
  it generates are alternately odd and even;
begin own integer array p, d[2: n]; integer k, q; real t;
  if first then initialize:
  begin for k := 2 step 1 until n do
    begin p[k] := 0; d[k] := 1 end;
    first := false
  end initialize;
  k := 0;
  INDEX: p[n] := q := p[n] + d[n];
    if q = n then
    begin d[n] := -1; go to LOOP end;
    if q ≠ 0 then go to TRANSPOSE;
    d[n] := 1; k := k + 1;
    LOOP: if n > 2 then begin
      comment Note that n was called by value;
      n := n - 1; go to INDEX end LOOP;
  Final exit: q := 1; first := true;
  TRANSPOSE: q := q + k; t := x[q];
    x[q] := x[q + 1]; x[q + 1] := t
end PERM:
```

CERTIFICATION OF ALGORITHM 115
PERM [H. F. Trotter, *Comm. ACM* (Aug. 1962)]

G. F. SCHRACK
University of Alberta, Calgary, Alb., Canada

PERM was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. Timing tests were carried out under the same conditions as for PERMUTATION (Algorithm 71) and PERMUTE (Algorithm 86).

PERM is indeed the fastest permutation generator so far encountered. For $n = 8$, PERM is 25% faster than PERMUTE (989 against 1316 sec.). The values for r_n are (for a definition of r_n, see Certification of Algorithm 71, *Comm. ACM*, Apr. 1962):

n	6	7	8
r_n	.92	.95	.98

CERTIFICATION OF ALGORITHM 115
PERM [H. F. Trotter, *Comm. ACM*, Aug. 1962]

E. S. PHILLIPS
Michigan State University, East Lansing, Mich.

PERM was translated into FORTRAN for the CDC 160-A, and it performed correctly. For $n = 8$, this method requires 2822 seconds. For comparison, Algorithm 86, *PERMUTE*, was translated and run on the same machine, requiring 3710 seconds as opposed to 1316 when run on an IBM 1620.

ALGORITHM 116
COMPLEX DIVISION
ROBERT L. SMITH
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```
procedure complexdiv (a, b, c, d) results: (e, f);
value a, b, c, d; real a, b, c, d;
comment complexdiv yields the complex quotient of a + ib
  divided by c + id. The method used here tends to avoid arith-
  metic overflow or underflow. Such spills could otherwise occur
  when squaring the component parts of the denominator if the
  usual method were used;
begin real r, den;
  if abs (c) ≧ abs (d) then
  begin r := d/c;
    den := c + r × d;
    e := (a + b × r)/den;
    f := (b − a × r)/den;
  end
  else
  begin r := c/d;
    den := d + r × c;
    e := (a × r + b)/den;
    f := (b × r − a)/den;
  end
end complexdiv
```

ALGORITHM 117
MAGIC SQUARE (EVEN ORDER)

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Elliott Brothers (London) Limited, Borehamwood, Herts., England

```
procedure magiceven (n, x); value n; integer array x; integer n;
comment the method of Devedec for even n is described in "Mathematical Recreations" by M. Kraitchik, pp. 150-2. Enter with side of square n to produce a magic square of the integers 1 - n ↑ 2 in x, where n ≧ 4;
begin integer a, b, n2, nn; Boolean p, q, r;
  n2 := n ÷ 2; nn := n × n;
  begin
procedure alpha (p, q, a, h); value p, q, a, h; integer p, q, a; Boolean h;
Comment pattern 0/0/0/ ··· ;
  begin integer r;
    for r := p step 1 until q do begin
      x[r, a] := if h then (a × n - n + r) else (nn - a × n + 1 + n - r); h := ¬h end;
end alpha;
procedure beta (p, q, a, h); value p, q, a, h; integer p, q, a; Boolean h;
comment pattern 1 - 1 - 1 - ··· ;
  begin integer r;
    for r := p step 1 until q do begin
      x[r, a] := if h then [nn - a × n + r) else (a × n + 1 - r); h := ¬ h end;
end beta;
procedure gamma (p, q, a, h); value p, q, a, h; integer p, q, a; Boolean h;
comment pattern /-/-/- ··· ;
  begin integer r;
    for r := p step 1 until q do begin
      x[r, a] := if h then (nn - a × n + n - r + 1) else (a × n + 1 - r); h := ¬ h end;
end gamma;
comment program begins;
p := q := (n -(n ÷ 4) × 4 = 0); r := true;
for a := 1 step 1 until (n2 - 1) do begin
  beta (1, a - 1, a, r); alpha (a, n2 - 1, a, true);
  x[n2, a] := if q then (nn - a × n + n2 + 1) else (nn - a × n + n2);
  alpha (n2 + 1, n, a, ¬ q);
  q := ¬ q; r := ¬ r end;
alpha (1, n2 - 1, n2, ¬ p); alpha (n2 + 2, n, n2, false);
gamma (1, n2 - 1, n2 + 1, p); gamma (n2 + 2, n, n2 + 1, true);
q := p; r := true;
for a := (n2 + 2) step 1 until n do begin
  beta (1, n - a, a, q); x[n - a + 1, a] := a × n - a + 1;
  beta (n - a + 2, n2 - 1, a, true);
  if r then for b := n2, n2 + 1 do x[b, a] := nn - a × n + n - b + 1
    else begin x[n2, a] := nn - a × n + n2;
      x[n2 + 1, a] := a × n - n2 + 1 end;
  beta (n2 + 2, a - 1, a, ¬ r); alpha (a, n, a, true);
  q := ¬ q; r := ¬ r end;
for a := n2, n2 + 1 do for b := n2, n2 + 1 do
  x[b, a] := if p then (a × n - n + b) else (nn - a × n + n - b + 1);
if ¬ p then begin
  for a := n2, n2 + 1 do x[n2 - 1, a] := a × n - n2 + 2;
  for b := n2, n2 + 1 do x[b, n2 + 2] := n × n2 - 2 × n + b end;
end end magiceven
```

CERTIFICATION OF ALGORITHMS 117 AND 118
MAGIC SQUARE (ODD AND, EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

D. M. COLLISON
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

Both algorithms were checked and timed, using a special ALGOL program, with the Elliott ALGOL translator on the National-Elliott 803. The procedure for odd orders was the slower:

Procedure	*Size of Square*	*Time*
Odd order	9	10 sec.
	19	45 sec.
Even order	10	7 sec.
	20	23 sec.

Because of the different methods used and the length of the even order procedure it was decided not to combine the two. The smallest square of even order generated is given below:—

13	3	2	16
8	10	11	5
12	6	7	9
1	15	14	4

CERTIFICATION OF ALGORITHMS 117 AND 118
MAGIC SQUARES (EVEN AND ODD ORDERS)

[D. M. Collison, [*Comm. ACM*, Aug. 1962]

P. NAUR
Regnecentralen, Copenhagen, Denmark

MAGICEVEN needed the following correction: Within the body of **procedure** beta a left square bracket: . . . **then** [*nn* . . . should be changed to a left parenthesis: . . . **then** (*nn* . . .

With this correction it has run successfully in the GIER ALGOL system. The squares of even orders from 4 to 20 were generated and checked for magicity in rows and columns, but not in diagonals.

The algorithm contains 11 pairs of superfluous parentheses (10 of which are in conditional expressions) and if the assignments to *n2* and *nn* are moved to the place just following "**end** gamma;" the inner block becomes unnecessary.

MAGICODD ran without correction in GIER ALGOL and produced a few reasonable-looking squares.

Run times are as follows:

Procedure	*Size of square*	*Time*
Magicodd	9	0.6 sec
	19	2.5 sec
Magiceven	10	0.9 sec
	20	2.3 sec

CERTIFICATIONS OF ALGORITHMS 117 and 118 MAGIC SQUARE (ODD AND EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

K. M. BOSWORTH
I.C.T. Ltd., Blyth Road, Hayes, Middlesex, England

The statement within the **Booleon procedure** *beta* should be changed from

$x[r,a]$:= **if** h **then** $[nn-a\times n+r)$ **else** $(a\times n+1-r)$;

to

$x[r,a]$:= **if** h **then** $(nn-a\times n+r)$ **else** $(a\times n+1-r)$;

The procedures were then tested on magic squares of order 3 to 17 inclusive without fault.

ALGORITHM 118
MAGIC SQUARE (ODD ORDER)

D. M. COLLISON
Elliott Brothers (London) Limited, Borehamwood, Herts., England

```
procedure magicodd (n, x); value n; integer n; integer
  array x;
comment for given side n the procedure generates a magic
  square of the integers 1 − n ↑ 2. For the method of De la
  Loubère, see M. Kraitchik, "Mathematical Recreations," p.
  149. n must be odd and n ≧ 3;
begin integer i, j, k;
  for i := 1 step 1 until n do
    for j := 1 step 1 until n do x[i, j] := 0;
  i := (n + 1) ÷ 2;  j := n;
  for k := 1 step 1 until n × n do begin
    if x[i, j] ≠ 0 then begin i := i − 1;  j := j − 2;
      if i < 1 then i := i + n;  if j < 1 then j := j + n end;
    x[i, j] := k;
    i := i + 1;  if i > n then i := i − n;
    j := j + 1;  if j > n then j := j − n;
    end;
end magicodd
```

CERTIFICATION OF ALGORITHMS 117 AND 118
MAGIC SQUARE (ODD AND, EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

D. M. COLLISON
Elliott Bros. (London) Ltd., Borehamwood, Herts., England

Both algorithms were checked and timed, using a special ALGOL program, with the Elliott ALGOL translator on the National-Elliott 803. The procedure for odd orders was the slower:

Procedure	*Size of Square*	*Time*
Odd order	9	10 sec.
	19	45 sec.
Even order	10	7 sec.
	20	23 sec.

Because of the different methods used and the length of the even order procedure it was decided not to combine the two. The smallest square of even order generated is given below:—

13	3	2	16
8	10	11	5
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CERTIFICATION OF ALGORITHMS 117 AND 118
MAGIC SQUARES (EVEN AND ODD ORDERS)

[D. M. Collison, [*Comm. ACM*, Aug. 1962]

P. NAUR
Regnecentralen, Copenhagen, Denmark

MAGICEVEN needed the following correction: Within the body of **procedure** beta a left square bracket: . . . **then** [*nn* . . . should be changed to a left parenthesis: . . . **then** (*nn* . . .

With this correction it has run successfully in the GIER ALGOL system. The squares of even orders from 4 to 20 were generated and checked for magicity in rows and columns, but not in diagonals.

The algorithm contains 11 pairs of superfluous parentheses (10 of which are in conditional expressions) and if the assignments to *n*2 and *nn* are moved to the place just following "**end** gamma;" the inner block becomes unnecessary.

MAGICODD ran without correction in GIER ALGOL and produced a few reasonable-looking squares.

Run times are as follows:

Procedure	*Size of square*	*Time*
Magicodd	9	0.6 sec
	19	2.5 sec
Magiceven	10	0.9 sec
	20	2.3 sec

CERTIFICATION OF ALGORITHM 118
MAGIC SQUARE (ODD ORDER) [D. M. Collison, *Comm. ACM*, Aug. 1962]

HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of the procedure *magicodd* was tested on the LGP-30 using the Dartmouth ALGOL 60 translator. No syntactical errors were found. The procedure generated odd-order magic squares satisfactorily. For orders up to 9, times were as follows (including output on the Flexowriter):

Order	*Time (sec)*
3	171
5	422
7	804
9	1285

The 3 × 3 square was:

4	3	8
9	5	1
2	7	6

CERTIFICATIONS OF ALGORITHMS 117 and 118
MAGIC SQUARE (ODD AND EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

K. M. BOSWORTH
I.C.T. Ltd., Blyth Road, Hayes, Middlesex, England

The statement within the **Booleon procedure** *beta* should be changed from

```
x[r,a] := if h then [nn−a×n+r) else (a×n+1−r);
```

to

```
x[r,a] := if h then (nn−a×n+r) else (a×n+1−r);
```

The procedures were then tested on magic squares of order 3 to 17 inclusive without fault.

ALGORITHM 119
EVALUATION OF A PERT NETWORK

BURTON EISENMAN AND MARTIN SHAPIRO
United Nuclear Corp., White Plains, N. Y.

```
procedure pert (nmax, i, j, te, st, emax, l, es, at);
comment An algorithm describing an iterative procedure for
  evaluating a PERT network that permits the use of arbitrarily
  ordered activities and event identifiers such that an upper
  triangular matrix type of solution is unnecessary.
    It has been observed by investigations of PERT networks,
  that an N × N matrix whose rows are designated as predecessor
  and whose columns are designated as successor events, has an
  entry in the (i, j)-element representing the activity time re-
  quired in going from event i to event j. By elementary transfor-
  mations, the matrix is transformed generally into an upper
  triangular matrix. The resultant upper triangular matrix is well
  ordered (i.e. any activity time appearing in a column is not
  dependent upon those activity times which appear in columns
  to the right of it).
    This precise manipulation generally demands considerable
  running time. By direct evaluation not requiring a collection of
  elementary transformations, it is possible to evaluate the net-
  work with considerable reduction of running time;
integer nmax, emax;
real st;
integer array i, j, l;
real array te, es, at;
comment Given the total number of activities, nmax, the pre-
  ceding and succeeding event identifiers, in and jn, the cor-
  responding expected time, te, for each activity, and the starting
  time, st, of the network, this procedure computes the early start
  and late finish times, es_e and at_e, for each event, l_e, in the net-
  work;
begin
procedure scan (e, t, l);
integer e, t;
integer array l;
comment Given the number of events, e−1, contained thus far
  in vector array, l, and an event identifier in or jn, stored in t,
  this procedure scans the existing array, l, to determine whether
  the event should be added to the list or not. If it is to be added,
  it becomes l_e and e replaces the event identifier. If it is not
  added, k replaces the event identifier.;
begin
integer k;
        if e = 1 then go to add;
        for k := e−1 step −1 until 1 do
begin   if t = l[k] then
begin   t := k;
        go to out
end
end;
add:    l[e] := t;
        t := e;
        e := e + 1;
out:
end scan;

integer n, e, s, t, k;
real    a, x;
        e := 1;
        for n := 1 step 1 until nmax do
begin   t := j[n];
        scan (e, t, l);
        j[n] := t;
        t := i[n];
        scan (e, t, l);
        i[n] := t
end;
comment By means of the switch, s, we will either compute the
  activity times, at_e, and transfer the values to the early start
  vector, es_e, or we will compute at_e without any transfer process,
  in which case the late finish times will be obtained.;
  emax := e − 1;
        s := 1;
        a := st;
s1:     k := emax;
        for e := 1 step 1 until emax do
        at[e] := a;
s2:     for n := 1 step 1 until nmax do
begin   if l[i[n]] > 0 then
begin   switch s := b1, b2;
b1:     x := abs (at[i[n]]) + te[n];
        if x > abs (at[j[n]]) then go to l1;
        go to l2;
b2:     x := abs (at[i[n]]) − te[n];
        if x < abs (at[j[n]]) then
l1:     at[j[n]] := − x;
l2:
end
end;
        for e := 1 step 1 until emax do
begin   if l[e] < 0 then
begin   if at[e] < 0 then
begin   l[e] := abs (l[e]);
        k := k + 1;
s3:     at[e] := abs (at[e]);
        go to l3
end;
        go to l3
end;
        if at[e] ≧ 0 then
begin   l[e] := − l[e];
        k := k − 1;
        go to l3
end;
        go to s3;
l3:
end;
        if k ≠ 0 then go to s2;
        switch s := g1, g2;
g1:     s := 2;
        for n := 1 step 1 until nmax do
begin   t := i[n];
        i[n] := j[n];
        j[n] := t
end;
```

```
        a := 0;
        for e := 1 step 1 until emax do
begin   es[e] := at[e];
        l[e] := abs (l[e]);
        if at[e] > a then
        a := at[e]
end;
        go to s1;
g2:     for e := 1 step 1 until emax do
        l[e] := abs (l[e]);
end pert
```

CERTIFICATION OF ALGORITHM 119 [H] EVALUATION OF A PERT NETWORK [Burton Eisenman and Martin Shapiro, *Comm. ACM 5* (Aug. 1962), 436]

L. STEPHEN COLES (Recd. 10 Nov. 1964 and 7 Dec. 1964)
Carnegie Institute of Technology, Pittsburgh, Pa.

The procedure was tested on a CDC-G20, using the ALGOL compiler developed by Carnegie Tech. Before compilation was possible, the following modifications were required in order to make it a correct ALGOL 60 procedure.

1. Insert after the end of *scan*
   switch *sw2* := *g1*, *g2*;
2. Modify **comment** By means of the switch, *s*, ···
to read
   comment By means of the switches, *sw1* and *sw2*, ···
3. Modify **begin switch** *s* := *b1*, *b2*;
to read
   begin switch *sw1* := *b1*, *b2*; **go to** *sw1* [*s*];
4. Modify **switch** *s* := *g1*, *g2*;
to read
   go to *sw2* [*s*];

With these changes the procedure was operated successfully on a number of small test problems.

ALGORITHM 120
MATRIX INVERSION II

RICHARD GEORGE*
Particle Accelerator Division Argonne National Laboratory Argonne, Illinois

* Work supported by the U. S. Atomic Energy Commission.

```
procedure INVERSION II (n, a, epsilon, ALARM, delta);
comment This is a revision of Algorithm 58. It accomplishes inversion of the matrix a, with the result stored in matrix a. The order of the matrix is n. If in the process of calculating, any pivot element has an absolute value less than epsilon, there will be a jump to the non-local label ALARM. The variable delta will contain the value of the determinant of the original matrix on normal exit, zero or a very small number on exit to ALARM.;
value n;
array a;
real epsilon, delta;
integer n;
begin
  array b, c[1:n]; real w, y;
  integer array z[1:n]; integer i, j, k, l, p;
  delta := 1.0;
  for j := 1 step 1 until n do
    z[j] := j;
  for i := 1 step 1 until n do
    begin
      k := i; y := a[i, i]; l := i-1; p := i+1;
      for j := p step 1 until n do
        begin
          w := a[i, j];
      if abs(w) > abs(y) then
        begin
          k := j;
          y := w
        end;
    end;
  delta := delta × y;
  if abs(y) < epsilon then go to ALARM;
  y := 1.0 / y;
  for j := 1 step 1 until n do
    begin
      c[j] := a[j, k];
      a[j, k] := a[j, i];
      a[j, i] := - c[j] × y;
      b[j] := a[i, j] := a[i, j] × y
    end;
  a[i, i] := y;
  j := z[i];
  z[i] := z[k];
  z[k] := j;
  for k := 1 step 1 until l, p step 1 until n do
    for j := 1 step 1 until l, p step 1 until n do
      a[k, j] := a[k, j] - b[j] × c[k]
        end;
  for i := 1 step 1 until n do
    begin
REPEAT: k := z [i];
          if k=i then go to ADVANCE;
          for j := 1 step 1 until n do
            begin
              w := a [i, j];
              a [i, j] := a [k, j];
              a [k, j] := w
            end;
          p := z [i];
          z [i] := z [k];
          z [k] := p;
          delta := - delta;
          go to REPEAT;
ADVANCE: end;
end
```

CERTIFICATION OF ALGORITHMS 120 AND MATRIX INVERSION BY GAUSS-JORDAN

INVERSION II [R. George, *Comm. ACM* Aug. 1962] and gjr [by H. Rutishauser, quoted by H. R. Schwarz, *Comm. ACM* Febr. 1962]

P. NAUR
Regnecentralen, Copenhagen, Denmark

These two procedures were compared using the GIER ALGOL system (30 bits for the normalized mantissa including sign). The following changes (in part dictated by the requirements of the compiler) were included:

INVERSION II: (1) Epsilon was included in the value part. (2) The specification **label** *ALARM* was added.

gjr: (1) The value part: **value** *n, eps* was inserted. (2) The second *a* in the formal parameter part was taken out.

With these changes both procedures ran smoothly through the compiler. In order to obtain a comparison each of them was tested as follows: With a given, rather large value of epsilon the procedure was called to invert a segment of the Hilbert matrix. Upon alarm exit, the value of epsilon was divided by 10 and a fresh call was made. In this way an estimate of the largest permissible epsilon was obtained. When the inverse had been obtained, that element of it which was most in error was found through a comparison with the accurate inverse as calculated by means of INVHILBERT (Algorithm 50, see certification above). A relative error was obtained through division by the largest element of the accurate inverse.

This process was carried out for segments of the Hilbert matrix of orders 2 through 15. For orders above 9, the results of the inversion are dominated by errors. Below 9 we obtained the following output:

Inversion by INVERSION II

Order	*eps*	*Determinant*	*Maximum error Subscr.*	*Maximum error Error*	*Maximum error Relative*
2	$10-2$	$8.3333333_{10}-2$	2,2	$2.98_{10}-8$	$2.48_{10}-9$
3	$10-3$	$4.6296284_{10}-4$	2,2	$5.01_{10}-5$	$2.61_{10}-7$
4	$10-4$	$1.6534314_{10}-7$	3,3	$3.06_{10}-2$	$4.72_{10}-6$
5	$10-5$	$3.7490001_{10}-12$	4,4	$1.38_{10}1$	$7.72_{10}-5$
6	$10-7$	$5.3601875_{10}-18$	5,5	$5.78_{10}3$	$1.31_{10}-3$
7	$10-8$	$4.8485529_{10}-25$	5,5	$3.70_{10}5$	$2.77_{10}-3$
8	$10-10$	$1.5221000_{10}-33$	6,6	$3.33_{10}9$	$7.84_{10}-1$

Similarly we got for gjr, and the ratio of errors of the two procedures:

		Inversion by gjr			Ratio of errors
		Maximum error		*Maximum error*	*INVERSION II*
Order	*eps*	*Subscr.*	*Error*	*Relative*	*to gjr*
2	$10-2$	2,1	$2.98_{10}-8$	$2.48_{10}-9$	1.0
3	$10-3$	2,2	$2.86_{10}-6$	$1.49_{10}-8$	18
4	$10-4$	4,3	$1.07_{10}-4$	$1.65_{10}-8$	290
5	$10-6$	4,4	2.48	$1.39_{10}-5$	5.6
6	$10-7$	5,5	$4.05_{10}3$	$9.18_{10}-4$	1.4
7	$10-8$	5,5	$4.32_{10}6$	$3.24_{10}-2$	.086
8	$10-10$	7,7	$5.55_{10}7$	$1.31_{10}-2$	60

Although the superiority of gjr, which searches for the pivot in both columns and rows, over INVERSION II, which only searches in the next column, is well brought out in the last column of the second table the behavior for $n = 7$ is curious and ought to be confirmed elsewhere.

As a further test both procedures were used to invert the matrices produced by Algorithm 52, TESTMATRIX (see certification above). Again, the error of the inverse was found by a comparison with the known inverse. The comparison of the two procedures was made for orders 2 through 23 and revealed a surprisingly small difference of accuracy. Typical output was as follows:

	Location and size of max. error				Ratio of errors
	INVERSION II		*gjr*		*INVERSION II*
Order	*Subscr.*	*Error*	*Subscr.*	*Error*	*to gjr*
5	5,5	$8.94_{10}-8$	5,5	$8.94_{10}-8$	1.00
10	10,10	$3.76_{10}-6$	10,10	$3.52_{10}-6$	1.07
15	15,15	$2.12_{10}-5$	15,15	$1.78_{10}-5$	1.19
20	20,20	$6.81_{10}-5$	20,20	$6.71_{10}-5$	1.02

The relative errors of the determinants calculated by INVERSION II increased slowly with n, reaching $2.3_{10}-7$ for $n = 24$.

Typical execution times were found as follows:

Order	*INVERSION II*	*gjr*
5	2 seconds	3 seconds
10	5 "	8 "
15	16 "	17 "
20	53 "	57 "

However, it should be noted that owing to the automatic segmentation of the program into drum tracks in GIER ALGOL the execution time may vary somewhat from one program in which a procedure is used to another. The above times do not, in fact, refer to the same program.

CORRECTION TO EARLIER REMARKS ON ALGORITHM 42 INVERT, ALG. 107 GAUSS'S METHOD, ALG. 120 INVERSION II, AND gjr [P. Naur, *Comm. ACM*, Jan. 1963, 38–40.]

P. NAUR
Regnecentralen, Copenhagen, Denmark

George Forsythe, Stanford University, in a private communication has informed me of two major weaknesses in my remarks on the above algorithms:

1) The computed inverses of rounded Hilbert matrices are compared with the exact inverses of unrounded Hilbert matrices, instead of with very accurate inverses of the rounded Hilbert matrices.

2) In criticizing matrix inversion procedures for not searching for pivot, the errors in inverting positive definite matrices cannot be used since pivot searching seems to make little difference with such matrices.

It is therefore clear that although the figures quoted in the earlier certification are correct as they stand, they do not substantiate the claims I have made for them.

To obtain a more valid criterion, without going into the considerable trouble of obtaining the very accurate inverses of the rounded Hilbert matrices, I have multiplied the calculated inverses by the original rounded matrices and compared the results with the unit matrix. The largest deviation was found as follows:

	Maximum deviation from elements of the unit matrix		
Order	*INVERSION II*	*gjr*	*Ratio*
2	$-1.49_{10}-8$	$-1.49_{10}-8$	1.0
3	$-4.77_{10}-7$	$-8.34_{10}-7$	0.57
4	$-9.54_{10}-6$	$-3.43_{10}-5$	0.28
5	$-7.32_{10}-4$	$-4.58_{10}-4$	1.6
6	$-1.61_{10}-2$	$-1.42_{10}-2$	1.1
7	$-5.78_{10}-1$	$-5.47_{10}-1$	1.1
8	$-1.20_{10}-2$	$-1.38_{10}1$	8.7
9	$-4.91_{10}1$	$-2.22_{10}1$	2.2

This criterion supports Forsythe's criticism. In fact, on the basis of this criterion no preference of INVERSION II or *gjr* can be made.

The calculations were made in the GIER ALGOL system, which has floating numbers of 29 significant bits.

ALGORITHM 121
NORMDEV
DAVID SHAFER
University of Chicago, Chicago, Ill.

```
procedure NormDev(Random,A,x);
  procedure Random; real A,x;
  comment 'NormDev' uses (1) a procedure 'Random(y)' assumed to produce a random number, 0 < y < 1, and (2) the constant A = sqrt(2/pi) × integral [0:1] exp(−x↑2/2)dx, to produce a positive normal deviate 'x';
  begin real y;
    Random(x); if x > A then go to large;
    x := x/A;
    1: Random(y); if y < exp(−x↑2/2) then go to EndND;
       Random(x); go to 1;
    large: x := (x − A)/(1 − A);
    2: x := sqrt(1 − 2 × log(x));
       Random(y); if y < 1/x then go to EndND;
       Random(x); go to 2;
  EndND: end
```

CERTIFICATION OF ALGORITHM 121 [G5]
NORMDEV

[David Shafer, *Comm. ACM 5* (Sept. 1962), 482]

M. C. PIKE (Recd. 3 May 1965)
Statistical Research Unit of the Medical Research Council, U. College Hospital Medical School, London.

Algorithm 121 has the following error: The line

```
2: x := sqrt (1 − 2 × log (x));
```

should read

```
2: x := sqrt (1 − 2 × ln (x));
```

With this correction *NormDev* has been run successfully on the ICT Atlas computer with the Atlas ALGOL compiler.

ALGORITHM 122
TRIDIAGONAL MATRIX

GERARD F. DIETZEL
Burroughs Corp., Pasadena, Calif.

```
procedure TRIDIAG (n,A,U);
integer n; array A,U;
comment This procedure reduces a real symmetric matrix A of
  order n to tridiagonal form (UT)AU (UT = transpose of U) by
  a sequence of at most (n-1)(n-2)/2 binary orthogonal trans-
  formations. Also, the matrix U is calculated. [Cf. W. Givens,
  "Numerical computation of the characteristic values of a real
  symmetric matrix," Report ORNL1574 (1954), Oak Ridge Nat.
  Lab., Tenn., and D. E. Johansen, "A modified Givens method
  for the eigenvalue evaluation of large matrices," J. ACM 8, 3
  (1961)];
begin real fact,c1,c2,loc1,loc2,temp; integer i,j,j1,j2,j3,j4,n1;
  comment Set array U = identity matrix of order n;
  for i := 1 step 1 until n do
  begin
    for j := i+1 step 1 until n do U[i,j] := U[j,i] = 0;
    U[i,i] := 1.0
  end;
  comment The reduction of the matrix A begins here. Only the
    upper triangular elements of A are used in the computation;
  n1 := n - 2;
  for i := 1 step 1 until n1 do
  begin
    j1 := i + 1; j2 := i + 2;
    for j := j2 step 1 until n do
    begin
      if A[i,j] = 0 then go to lab;
      fact := 1 / sqrt(A[i,j1]↑2 + A[i,j]↑2);
      c1 := fact × A[i,j1]; c2 := fact × A[i,j];
      loc1 := A[j1,j1]; loc2 := A[j1,j];
      A[j1,j1] := c1↑2 × loc1 + 2.0 × c1 × c2 × loc2 + c2↑2 ×
        A[j,j];
      A[j1,j] := -c1 × c2 × loc1 + (c1↑2 - c2↑2) × loc2 + c1 ×
        c2 × A[j,j];
      A[j,j] := c2↑2 × loc1 - 2.0 × c1 × c2 × loc2 + c1↑2 ×
        A[j,j];
      j3 := j + 1;
      for k := j3 step 1 until n do
      begin
        temp := A(j1,k];
        A[j1,k] := c1 × temp + c2 × A[j,k];
        A[j,k] := -c2 × temp + c1 × A[j,k]
      end;
      j4 := j - 1;
      for k := j2 step 1 until j4 do
      begin
        temp := A[j1,k];
        A[j1,k] := c1 × temp + c2 × A[k,j];
        A[k,j] := -c2 × temp + c1 × A[k,j]
      end;
      A[i,j1] := c1 × A[i,j1] + c2 × A[i,j];
      A[i,j] := 0;
      for k := 1 step 1 until n do
      begin
        temp := U[k,j1];
        U[k,j1] := c1 × temp + c2 × U[k,j];
        U[k,j] := -c2 × temp + c1 × U[k,j]
      end;
lab:  end
  end;
  for i := 1 step 1 until n do
    for j := i+1 step 1 until n do
      A[j,i] := A[i,j]
end TRIDIAG
```

CERTIFICATION OF ALGORITHM 122
TRIDIAGONAL MATRIX [Gerard F. Dietzel, *Comm. ACM 5* (Sept. 1962), 482]

PETER NAUR (Recd 27 Sept. 63)
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TRIDIAG needed the following corrections:

1. Insert *k* among the local integers to read:
   integer *i, j, j1, j2, j3, j4, n1, k*;
2. At the end of line 5 of the procedure body, insert the colon to read *U[j, i]* := 0;
3. Change the round parenthesis to a square bracket following **for** *k* := *j3* ··· to read *temp* := *A[j1, k]*;

With these corrections the algorithm worked satisfactorily with the GIER ALGOL system. As a test it was tried with the following matrix:

$$HBH\ TESTMATRIX[j, i] = HBH\ TESTMATRIX[i, j]$$
$$= n + 1 - j \qquad (j \geqq i)$$

(cf. the Certification of Alg. 85, *Comm. ACM 6* (Aug. 1963), 447). As a check the resulting matrix was rotated back again, using the resulting *U*-matrix, and the largest deviation of any element from the original was found.

For comparison the figures obtained by using the algorithms given by Wilkinson in *Numerische Mauhematik 4* (1962), 354–376, may be used. Wilkinson's algorithms use Householder's method of obtaining the tridiagonal form. It should be noted that the deviations given in the table below for Householder's method refer to the final result of obtaining the eigenvalues and vectors, and not only the tridiagonal form, and thus include error contributions from a rather longer chain of calculations than the ones given for *TRIDIAG*. The times, however, only refer to the tridiagonalisation process in both cases.

	$n=5$	$n=10$	$n=15$
Largest deviation			
TRIDIAG,	$1.4_{10}-7$	$7.0_{10}-7$	$2.4_{10}-6$
householder tridiagonalisation		$1.4_{10}-7$	$1.3_{10}-6$
Time of execution, in GIER ALGOL, seconds			
TRIDIAG	2	7	34
householder tridiagonalisation	1	4	10

These figures clearly demonstrate the superiority of the Householder process. Since, in addition, the Householder method in the form given by Wilkinson uses much less storage for variables, Algorithm 122 cannot be recommended.

ALGORITHM 123
REAL ERROR FUNCTION, ERF(x)

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```
real procedure Erf(x); real x;
comment Φ(x) = Erf(x) = (2/√π)∫₀ˣ e^(-u²) du can be computed
  by using the recursive relation for derivatives with Φ¹(x) =
  (2/√π)e^(-x²), where Φ^(n)(x) = -2xΦ^(n-1)(x) - 2(n-2)Φ^(n-2)(x),
  for n = 2, 3, ··· . The Taylor's series expansions of Φ(a_k) are
  taken about k+1 points on the interval 0 < a_k ≦ x and summed
  to get Φ(x);
begin real A, U, V, W, Y, Z, T; integer N;
      Z := 0; 1: if x ≠ 0 then
begin if 0.5 < abs (x) then A := - sign (x) × 0.5
      else A := - x;
      U := V := 1.12837917 × exp(-x↑2); Y := T := -V ×
        A; N := 1;
2:    if abs(T) ≧ 10- 10 then
begin N := N + 1; W := -2 × x × V - 2 × U × (N-2);
        T := T × W × A/(V × N);
      U := V; V := W; Y := Y + T; go to 2 end;
      Z := Z + Y; x := x + A; go to 1 end;
      Erf := Z end Erf
```

CERTIFICATION OF ALGORITHM 123
REAL ERROR FUNCTION, ERF (x) [Martin Crawford and Robert Techo, *Comm. ACM*, Sept. 1962]

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* Work supported by the U. S. Atomic Energy Commission.

The body of *Erf*(x) was tested using the Dartmouth SCALP compiler for the LGP-30. For $x = 0(0.01)0.3$, the results agreed with tabulated values to 8 in the 7th decimal place, and for $x = 0.4(0.2)1.6$ the error was less than 1 in the 6th decimal. These results are compatible with the roundoff error in the arithmetic used. The computing time increased rapidly (by a factor of more than 10) as x increased from 0.01 to 1.6.

The following comments should be considered by users of the algorithm:

1. The parameter x should be called by value, both to allow the use of expressions, and also to avoid destruction of the actual parameter.
2. The constant $_{10}-10$ in statement 2 determines the accuracy of the computation. Its value should be adjusted to the arithmetic being used, and the accuracy required. A machine-independent test could be made by substituting **if** $Y - T = Y$ **then** ··· .
3. For large x, the error function is more efficiently calculated from the Laplace continued fraction for $erfc(x)$. Algorithm 180 is based on this method.

REMARK ON ALGORITHM 123
ERF(x) [Martin Crawford and Robert Techo, *Comm. ACM*, Sept. 1962]

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(1) The specification **value** x; was added to allow x to be an expression and to prevent side effects.

(2) The algorithm was then modified to give the Gaussian integral $(1/\sqrt{2\pi})\int_{-\infty}^{x} \exp(-\frac{1}{2}u^2)\,du$ by

(a) changing its name to *Gauss* (x),

(b) inserting $x := x*0.70710678;$ immediately before $Z := 0;$, and

(c) changing the final statement to
Gauss := $(Z+1)/2$ **end** *Gauss*

(3) The algorithm with the above changes was tested on a National Elliott 803 computer using the Elliott-ALGOL translator with $_{10}-8$ substituted for $_{10}-10$. It was found to produce wrong answers when $x = \pm 1$ (corresponding to $Erf(\pm 1/\sqrt{2})$) giving 0.5 ± 0.3467899 instead of 0.5 ± 0.3413447.

REMARK ON ALGORITHM 123
ERF(x) [Martin Crawford and Robert Techo, *Comm. ACM* 5 (Sept. 1962), 483; 6 (June 1963), 316; 6 (Oct. 1963), 618]

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This algorithm may err when the Taylor series expands about a root of the nth-order Hermite polynomial; one such error has already been noted [Remark on Algorithm 123, D. Ibbetson, *Comm. ACM* 6 (Oct. 1963), 618]. The difficulty springs from the Taylor-series truncation criterion, which assumes that the magnitude of successive terms in the Taylor series decreases. This is not always so, as may be seen by relating

$$\Phi^{(n)}(x) \equiv \frac{2}{\sqrt{\pi}} \frac{d^{n-1}}{dx^{n-1}} (e^{-x^2}), \qquad (n \geqq 1)$$

to the Hermite polynomial $H_n(x)$, which can be defined as

$$H_n(x) \equiv (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}).$$

Therefore

$$\Phi^{(n)}(x) = \frac{2}{\sqrt{\pi}} (-1)^{n-1} e^{-x^2} H_{n-1}(x).$$

As a result, $\Phi^{(n)}(x)$ vanishes when x is a root of $H_{n-1}(x)$ and the Taylor series may be terminated prematurely.

The algorithm was translated into FORTRAN II and run on a Scientific Data Systems 910 computer (39-bit mantissa) with the following changes:

(1) The argument was decremented by 0.25 rather than 0.5.

(2) The truncation criterion for $abs\,(T)$ was 10^{-12} rather than 10^{-10}.

Errors, detected for $x = 1/\sqrt{2}$ and $x = 2.652$, were traced to the above described premature truncation of the relevant Taylor series. These arguments correspond to the roots of $H_2(x)$ and $H_7(x)$.

The program was therefore modified to sum a fixed number of terms, with special attention to the difficulties that might arise when expanding about roots of $H_n(x)$. In particular, in Algorithm 123, line 9, the coefficient, $A^n/n!$, of the nth term in the Taylor expansion, is obtained via the intermediate step of dividing the $(n-1)$-term, T, by the $(n-1)$-derivative, V. The possibility of dividing by $V = 0$ when the Taylor expansion takes place about roots of $H_{n-2}(x)$ was avoided by modifying the program to compute coefficients directly from the recursion relation,

$$A^n/n! = [A^{n-1}/(n-1)!][A/n].$$

In selecting the number of terms to be included in each Taylor series, consideration should also be given to the size of the standard decrement (specified as 0.5 in line 3 of Algorithm 123), for it is the combination of these two parameters which largely determines the accuracy and running time. A brief survey suggested that at least 10-digit accuracy could be obtained if a decrement of 0.4 were employed with 16 terms in each Taylor series; this resulted in an average running time of about 3.5 seconds per computation for arguments in the range $0 \leqq x \leqq 5.0$.

REFERENCE: H. MARGENAU and G. M. MURPHY, *The Mathematics of Physics and Chemistry*, pp. 119, 122. D. van Nostrand, 1943.

REMARKS ON:
ALGORITHM 123 [S15]
REAL ERROR FUNCTION, ERF(x)

[Martin Crawford and Robert Techo *Comm. ACM 5* (Sept. 1962), 483]

ALGORITHM 180 [S15]
ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 314]

ALGORITHM 181 [S15]
COMPLEMENTARY ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 315]

ALGORITHM 209 [S15]
GAUSS

[D. Ibbetson. *Comm. ACM 6* (Oct. 1963), 616]

ALGORITHM 226 [S15]
NORMAL DISTRIBUTION FUNCTION

[S. J. Cyvin. *Comm. ACM 7* (May 1964), 295]

ALGORITHM 272 [S15]
PROCEDURE FOR THE NORMAL DISTRIBUTION FUNCTIONS

[M. D. MacLaren. *Comm. ACM 8* (Dec. 1965), 789]

ALGORITHM 304 [S15]
NORMAL CURVE INTEGRAL

[I. D. Hill and S. A. Joyce. *Comm. ACM 10* (June 1967), 374]

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These algorithms were tested on the ICT Atlas computer using the Atlas ALGOL compiler. The following amendments were made and results found:

ALGORITHM 123

(i) **value** x; was inserted.

(ii) $abs(T) \leqslant_{10} -10$ was changed to $Y - T = Y$ both these amendments being as suggested in [1].

(iii) The labels 1 and 2 were changed to $L1$ and $L2$, the **go to** statements being similarly amended.

(iv) The constant was lengthened to 1.12837916710.

(v) The extra statement $x := 0.707106781187 \times x$ was made the first statement of the algorithm, so as to derive the normal integral instead of the error function.

The results were accurate to 10 decimal places at all points tested except $x = 1.0$ where only 2 decimal accuracy was found, as noted in [2]. There seems to be no simple way of overcoming the difficulty [3], and any search for a method of doing so would hardly be worthwhile, as the algorithm is slower than Algorithm 304 without being any more accurate.

ALGORITHM 180

(i) $T := -0.56418958/x/exp(v)$ was changed to $T := -0.564189583548 \times exp(-v)/x$. This is faster and also has the advantage, when v is very large, of merely giving 0 as the answer instead of causing overflow.

(ii) The extra statement $x := 0.707106781187 \times x$ was made as in (v) of Algorithm 123.

(iii) **for** $m := m + 1$ was changed to **for** $m := m + 2$. $m+1$ is a misprint, and gives incorrect answers.

The greatest error observed was 2 in the 11th decimal place.

ALGORITHM 181

(i) Similar to (i) of Algorithm 180 (except for the minus sign).

(ii) Similar to (ii) of Algorithm 180.

(iii) m was declared as **real** instead of **integer**, as an alternative to the amendment suggested in [4].

The results were accurate to 9 significant figures for $x \leqslant 8$, but to only 8 significant figures for $x = 10$ and $x = 20$.

ALGORITHM 209

No modification was made. The results were accurate to 7 decimal places.

ALGORITHM 226

(i) $10 \uparrow m/(480 \times sqrt(2 \times 3.14159265))$ was changed to $10 \uparrow m \times 0.00083129750836$.

(ii) **for** $i := 1$ **step** 1 **until** $2 \times n$ **do** was changed to $m := 2 \times n$; **for** $i := 1$ **step** 1 **until** m **do**.

(iii) $-(i \times b/n) \uparrow 2/8$ was changed to $-(i \times b/n) \uparrow 2 \times 0.125$.

(iv) **if** $i = 2 \times n - 1$ was changed to **if** $i = m - 1$

(v) $b/(6 \times n \times sqrt(2 \times 3.14159265))$ was changed to $b/(15.0397696478 \times n)$.

Tests were made with $m = 7$ and $m = 11$ with the following results:

x	*Number of significant figures correct*		*Number of decimal places correct*	
	$m = 7$	$m = 11$	$m = 7$	$m = 11$
−0.5	7	11	7	11
−1.0	7	10	7	10
−1.5	7	10	8	10
−2.0	7	9	8	10
−2.5	6	9	8	11
−3.0	6	7	8	9
−4.0	5	7	10	11
−6.0	2	1	12	10
−8.0	0	0	11	9

Perhaps the comment with this algorithm should have referred to decimal places and not significant figures. To ask for 11 significant figures is stretching the machine's ability to the limit, and where 10 significant figures are correct, this may be regarded as acceptable.

ALGORITHM 272

The constant .99999999 was lengthened to .9999999999.

The accuracy was 8 decimal places at most of the points tested, but was only 5 decimal places at $x = 0.8$.

ALGORITHM 304

No modification was made. The errors in the 11th significant figure were:

abs(x)	$x > 0 \equiv$ *upper*	$x > 0 \not\equiv$ *upper*
0.5	1	1
1.0	1	2
1.5	21[a](5)	2
2.0	25[a](0)	4
3.0	0	0
4.0	2	3
6.0	6	0
8.0	14	0
10.0	23	0
20.0	35	0

[a] Due to the subtraction error mentioned in the comment section of the algorithm. Changing the constant 2.32 to 1.28 resulted in the figures shown in brackets.

To test the claim that the algorithm works virtually to the accuracy of the machine, it was translated into double-length instructions of Mercury Autocode and run on the Atlas using the EXCHLF compiler (the constant being lengthened to 0.39894228040143267793994 6). The results were compared with hand calculations using Table II of [5]. The errors in the 22nd significant figure were:

abs(x)	$x > 0 \equiv$ *upper*	$x > 0 \not\equiv$ *upper*
1.0	2	3
2.0	7	1
4.0	2	0
8.0	8	0

Timings. Timings of these algorithms were made in terms of the Atlas "Instruction Count," while evaluating the function 100 times. The figures are not directly applicable to any other computer, but the relative times are likely to be much the same on other machines.

INSTRUCTION COUNT FOR 100 EVALUATIONS

abs(x)	Algorithm number							
	123	180	181	209	226 $m = 7$	272	304[a]	304[b]
0.5	58			8	97	24	25	24
1.0	65[c]			8	176	24	29	29
1.5	164	128	127	9	273	25	35	35
2.0	194	78	90	8	387	24	39	39
2.5	252	54	68	10	515	24	131	44
3.0		42	51	9	628	25	97	50
4.0		27	39	9	900[d]	25	67	44
6.0		15	30	6	1400[d]	16	49	23
8.0		9	28	7	2100[d]	18	44	11
10.0		10	25	5	2700[d]	16	38	11
20.0		9	22	5	6500[d]	16	32	11
30.0		9	9	5	10900[d]	16	11	11

[a] Readings refer to $x > 0 \equiv$ *upper*.

[b] Readings refer to $x > 0 \not\equiv$ *upper*.

[c] Time to produce incorrect answer. A count of 120 would fit a smooth curve with surrounding values.

[d] 100 times Instruction Count for 1 evaluation.

Opinion. There are advantages in having two algorithms available for normal curve tail areas. One should be very fast and reasonably accurate, the other very accurate and reasonably fast. We conclude that Algorithm 209 is the best for the first requirement, and Algorithm 304 for the second.

Algorithms 180 and 181 are faster than Algorithm 304 and may be preferred for this reason, but the method used shows itself in Algorithm 181 to be not quite as accurate, and the introduction of this method solely for the circumstances in which Algorithm 180 is applicable hardly seems worth while.

Acknowledgment. Thanks are due to Miss I. Allen for her help with the double-length hand calculations.

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ALGORITHM 124
HANKEL FUNCTION

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```
procedure HANKEL(N,X,H); value N,X; integer N;
  real X; array H;
comment This procedure evaluates the complex valued hankel
  function of the first kind for real argument X and integral order
  N and assigns it to H. The individual Bessel- and Neuman-func-
  tion series are not evaluated separately. Both the real and
  imaginary parts are generated from the same terms;
begin real K, P, R, A, S, T, D, L; integer Q;
  A := R := 1; H[1] := H[2] := S := 0;
  for Q := 1 step 1 until N do begin R := R × Q; S := S +
    1/Q end; D := R/N;
  R := 1/R; K := X × X/4; P := (X/2)↑N; T := ln(K) +
    1.1544313298631;
  for Q := 0, Q+1 while Q≦N∨L≠H[2] do
  begin L := H[2]; H[1] := H[1] + A×K×R;
    H[2] := H[2] + A×(R×K×(T−S) − (if Q<N then D/P
      else 0));
    A := A×K/Q; R := −R/(Q+N); S := S+1/Q + 1/(Q+N);
    if Q<N then D := D/(N−Q)
  end; H[2] := H[2] × .31830989
end
```

CERTIFICATION OF ALGORITHM 124 [S17]
HANKEL FUNCTION [Luis J. Schaeffer, *Comm. ACM 5* (Sept. 1962), 483]

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This procedure, after modification, was run on the B-5000 using B-5000 ALGOL. Values obtained checked with US National Bureau of Standards *Handbook of Mathematical Functions*, Applied Mathematics Series 55, US Government Printing Office, Washington, D.C. 1964.

For $N = 0$, 1 and 2, accuracy was to 10 decimals for $X < 8.0$. It deteriorated to 6 decimals for $8 < X < 17.5$. For $3 \leq N \leq 9$ accuracy was to the 5 decimals of the tables.

Some changes proved necessary to make the algorithm run. Since the algorithm is short and the changes are involved, the algorithm is restated here. Note that a test for a zero argument X is included in the body of the procedure since $H[2]$ ought to be minus infinity when $X = 0$.

```
procedure HANKEL (N, X, H); value N, X; integer N;
  real X; array H;
begin real K, P, R, A, S, T, D, L; integer Q;
  if X = 0 then
  begin comment In this case H[2] is minus infinity. M denotes
      the largest number which can be represented in the machine.
      The numerical value of M is to be written into the
      procedure:
    H[2] := −M;
    H[1] := if N = 0 then 1 else 0;
    go to exit
  end;
  A := R := 1; H[1] := H[2] := S := 0;
  if N = 0 then begin R := 1; S := D := 0 end
  else
  begin for Q := 1 step 1 until N do
    begin R := R × Q; S := S + 1/Q end; D := R/N
  end;
  R := 1/R; K := X × X/4; P := K ↑ N; T := ln (K) +
    1.1544313298631;
comment The last constant is 2 × gamma, Euler's constant;
for Q := 0, Q + 1 while Q ≤ N ∨ L ≠ H [2] do
begin L := H[2]; H[1] := H[1] + A × R;
  H[2] := H[2] + A × (R×(T−S) − (if q<N then D/P else 0));
  A := A × K/(Q+1); R := −R/(Q+N+1);
    S := S + 1/(Q+1) + 1/(Q+N+1);
    if Q + 1 < N then D := D/(N−Q−1);
  end;
  P := (X/2) ↑ N; H[1] := H[1] × P; H[2] := 0.318309886184
    × H[2] × P;
  comment The multiplicative constant is 1/Pi;
exit:
end HANKEL
```

ALGORITHM 125
WEIGHTCOEFF
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```
procedure weightcoeff (n,q,e,eps,w,x); value n; real eps;
          integer n; array q,e,w,x;
comment Computes abscissae x_i and weight coefficients w_i for
a Gaussian quadrature method ∫_0^b w(x)f(x) dx ≈ Σ_{i=1}^n w_i f(x_i),
where ∫_0^b w(x) dx = 1 and w(x) ≧ 0. The method requires the order
n, a tolerance eps and the 2n−1 first coefficients of the continued
fraction
```

$$\int_0^b \frac{w(x)}{z-x}\,dx = \cfrac{1}{z} - \cfrac{q_1}{1} - \cfrac{e_1}{z} - \cfrac{q_2}{1} - \cfrac{e_2}{z} - \cdots$$

```
to be given, the latter as two arrays q[1:n] and e[1:n−1] all com-
ponents of which are automatically positive by virtue of the con-
dition w(x) ≧ 0. The method works as well if the upper bound b
is actually infinity (note that b does not appear directly as param-
eter!) or if the density w(x) dx is replaced by dα(x) with a mono-
tonically increasing α(x) with at least n points of variation. The
tolerance eps should be given in accordance to the machine ac-
curacy, e.g. as 10−10 for a computer with a ten-digit mantissa. The
result is delivered as two arrays w[1:n] (the weight coefficients)
and x[1:n] (the abscissae). For a description of the method see
H. Rutishauser, "On a modification of the QD-algorithm with
Graeffe-type convergence" [Proceedings of the IFIPS Congress,
Munich, 1962].;
begin
  integer k;
  Boolean test;
  real m, p;
  array g[1:n];
  procedure red (a,f,n); value n; integer n; array a,f;
    comment subprocedure red reduces a heptadiagonal matrix
      a to tridiagonal form as described in the paper loc. cit. Since
      the bulk of the computing time of the whole method is spent
      in this subprocedure, it would pay to write it in machine
      code.;
  begin
    real c; integer j,k;
    for k := 1 step 1 until n−1 do
    begin
      for j := k step 1 until n−1 do
      begin
        c := −f[j] × a[j,7]/a[j,2];
        a[j,7] := 0;
        a[j+1,2] := a[j+1,2] + c × a[j,5];
        a[j,1] := a[j,1] − c × f[j]×a[j,4];
        a[j,6] := a[j,6] − c × a[j+1,1];
        a[j+1,3] := a[j+1,3] − c × a[j+1,6];
      end j;
      for j := k step 1 until n−1 do
      begin
        c := −f[j] × a[j,4]/a[j,1];
        a[j,4] := 0;
        a[j+1,1] := a[j+1,1] + c × a[j,6];
        a[j+1,6] := a[j+1,6] + c ×◦a[j+1,3];
        a[j,5] := a[j,5] − c × a[j+1,2];
        a[j+1,0] := a[j+1,0] − c × a[j+1,5];
      end j;
      for j := k+1 step 1 until n−1 do
      begin
        c := −a[j,3]/a[j−1,6];
        a[j,3] := 0;
        a[j,6] := a[j,6] + c × a[j,1];
        a[j−1,5] := a[j−1,5] − c × f[j] × f[j] × a[j,0];
        a[j,2] := a[j,2] − c × f[j] × f[j] × a[j,5];
        a[j,7] := a[j,7] − c × f[j] × a[j+1,2];
      end j;
      for j := k+1 step 1 until n−1 do
      begin
        c := −a[j,0]/a[j−1,5];
        a[j,0] := 0;
        a[j+1,2] := a[j+1,2] + c × f[j] × a[j,7];
        a[j,5] := a[j,5] + c × a[j,2];
        a[j,1] := a[j,1] − c × f[j] × f[j] × a[j,6];
        a[j,4] := a[j,4] − c × f[j] × a[j+1,1];
      end j;
    end k;
  end red;
  procedure qdgraeffe (n,h,g,f); value n;
    integer n; array h,g,f;
    comment Subprocedure qdgraeffe computes for a given
      finite continued fraction
```

$$f(z) = \cfrac{1}{z} - \cfrac{q_1}{1} - \cfrac{e_1}{z} - \cfrac{q_2}{1} - \cdots - \cfrac{q_n}{1}$$

```
    another one, the poles of which are the squares of the poles of
    f(z). However qdgraeffe uses not the coefficients q_1 , ··· , q_n
    and e_1 , ··· , e_{n−1} of f(z), but the quotients
```

$$\left.\begin{matrix} f_k = q_{k+1}/q_k \\ g_k = e_k/q_{k+1} \end{matrix}\right\} \qquad (k := 1,2,\cdots,n-1)$$

```
    and the h_k = ln(abs(q_k)) (k := 1,2,···,n), and the results are
    delivered in the same form. Procedure qdgraeffe can be used
    independently, but requires subprocedure red above;
  begin
    integer k; array a[0:n,0:7];
    g[n] := f[n] := 0;
    for k := 1 step 1 until n do
    begin
      a[k−1,4] := a[k−1,5] := 1;
      a[k,1] := a[k,2] := 1 + g[k] × f[k];
      a[k,6] := a[k,7] := g[k];
      a[k,0] := a[k,3] := 0;
      comment The array a represents the heptadiagonal
        matrix Q of the paper loc. cit., but with the modifications
        needed to avoid the large numbers and with a peculiar
        arrangement.;
    end k;
    a[n,5] := 0;
    red(a,f,n);
    for k := 1 step 1 until n do
      h[k] := 2 × h[k] + ln(abs(a[k,1] × a[k,2]));
      comment A saving might be achieved by economizing the
        log-computation in the range .8 ≦ x ≦ 1.2;
    for k := 1 step 1 until n−1 do
    begin
```

```
      f[k] := f[k] × f[k] × a[k+1,2] × a[k+1,1]/(a[k,1] × a[k,2]);
      g[k] := a[k,5] × a[k,6]/(a[k+1,1] × a[k+1,2])
    end k;
  end qdgraeffe;
L1: x[1] := q[1] + e[1];
    for k := 2 step 1 until n do
    begin
      g[k-1] := e[k-1] × q[k]/x[k-1];
      x[k] := q[k] + (if k=n then 0 else e[k]) - g[k-1];
      g[k-1] := g[k-1]/x[k];
      w[k-1] := x[k]/x[k-1];
      x[k-1] := ln(x[k-1]);
    end k;
    x[n] := ln(x[n]);
L2: p := 1;
L25: begin
       test := true;
       for k := 1 step 1 until n-1 do
         test := test ∧ abs(g[k] × w[k]) < eps;
       if test then go to L3;
       qdgraeffe (n,x,g,w);
     end;
     p := 2 × p;
     go to L25;
     comment What follows is a peculiar method to compute
       the w_k from given ratios g_k = w_{k+1}/w_k such that Σ_{k=1}^{n} w_k = 1,
       but the straightforward formulae to do this might well
       produce overflow of exponent.;
L3: w[1] := m := 0;
    for k := 1 step 1 until n-1 do
    begin
      w[k+1] := w[k] + ln(g[k]);
      if w[k] > m then m := w[k];
    end k;
    for k := 1 step 1 until n do w[k] := exp(w[k]-m);
    m := 0;
    for k := 1 step 1 until n do m := m + w[k];
    for k := 1 step 1 until n do begin w[k] := w[k]/m;
      x[k] := exp(x[k]/p) end;
end weightcoeff
```

ALGORITHM 126
GAUSS' METHOD
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```
procedure gauss (u,a,y);
real array a,y; integer u;
comment This procedure is for solving a system of linear equa-
  tions by successive elimination of the unknowns. The augmented
  matrix is a and u is the number of unknowns. The solution vector
  is y. If the system hasn't any solution or many solutions, this is
  indicated by the go to error where error is a label outside the
  procedure.;
  begin
      integer i,j,k,m,n;
      n := 0;
ck0:  n := n + 1;
      for k := n step 1 until u do if a[k,n] ≠ 0 then go to ck1;
      go to error;
ck1:  if k = n then go to ck2;
      for m := n step 1 until u+1 do
  begin
      temp := a[n,m]; a[n,m] := a[k,m]; a[k,m] := temp
  end;
ck2:  for j := u + 1 step -1 until n do a[n,j] := a[n,j]/a[n,n];
      for i := k + 1 step 1 until u do
      for j := n + 1 step 1 until u + 1 do
      a[i,j] := a[i,j] - a[i,n] × a[n,j];
      if n≠u then go to ck0;
      for i := u step -1 until 1 do
  begin
    y[i] := a[i,u + 1]/a[i,i];
    for k := i - 1 step -1 until 1 do
    a[k,u + 1] := a[k,u + 1] - a[k,i] × y[i]
  end end;
```

ALGORITHM 127
ORTHO

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```
procedure ORTHO(W,Y,Z,n,fn,m,p,r,ai,aui,mui,zei,X,DEV,
  COF,STD,CV,VCV,gmdt,Q,Q2,E,EP,A,GF,ENF);
value n,m,p,r,ai,aui,mui,zei;
real fn,gmdt;
array W,Y,Z,X,DEV,COF,STD,CV,VCV,Q,Q2,E,EP,A,GF,ENF;
integer n,m,p,r,ai,aui,zei,mui;
switch at := at1,at2; switch ze := ze1, ze2;
switch au := au1,au2; switch mu := mu1, mu2, mu3;
```

comment *ORTHO* is a general purpose procedure which is capable of solving a wide variety of problems. For a detailed discussion of the applications listed below and other applications, see (1) Philip Davis and Philip Rabinowitz, "A Multiple Purpose Orthonormalizing Code and Its Uses," *J. ACM 1* (1954), 183–191, (2) Philip Davis, "Orthonormalizing Codes in Numerical Analysis," in J. Todd (Ed.), *A Survey of Numerical Analysis*, Ch. 10 (McGraw-Hill, 1962), (3) Philip Davis and Philip Rabinowitz, "Advances in Orthonormalizing Computation," in F. L. Alt (Ed.), *Advances in Computers*, Vol. 2, pp. 55–133 (Academic Press, 1961), (4) Philip J. Walsh and Emilie V. Haynsworth, General Purpose Orthonormalizing Code, SHARE Abstr. #850. APPLICATIONS: (a) orthonormalizing a set of vectors with respect to a general inner product, (b) least squares approximation to given functions by polynomial approximations or any linear combination of powers, rational functions, transcendental functions and special functions, such as those defined numerically by a set of values, (c) curve fitting of empirical data in two or more dimensions, (d) finding the best solution in the l.s.s. to a system of m linear equations in n unknowns ($n \leqq m$), (e) matrix inversion and solution of linear systems of equations, (f) expansion of functions in a series of orthogonal functions, such as a series of Legendre or Chebyshev polynomials.

The following information must be supplied to the procedure. (We are considering here the approximation feature of the procedure.)

n the number of components per vector (excluding augmentation)

m the number of vectors used in the approximation. For a polynomial fit of degree t, set $m=t+1$.

p the number of augmented components per vector. A feature of this procedure is that once the approximating vectors nave been orthonormalized, they may be used in approximating r functions without repeating the orthonormalization procedure on the original approximating vectors.

r the number of functions to be approximated.

ai a switch control concerning the approximating vectors. With $ai=1$, the procedure selects the first n components of the first row of $[Z]$, supplied by user. The i powers of these values are computed and stored into working location $[X]$, $i=0(1)m-1$. This is the usual set up for a polynomial fit. With $ai=2$, the procedure selects the first n components of the first m rows of $[Z]$ supplied by user and stores them into working location $[X]$.

aui a switch control concerning augmentation on the approximating vectors. If $p=0$, this switch is ignored. With $aui=1$, regular augmentation is applied to the vectors in $[X]$. p zeros are stored after the nth component of the first m rows of $[X]$. The $(n+i)$th component is replaced by 1.0, $i=1(1)m$. With $aui=2$, special augmentation is applied to the vectors in $[X]$. The p components located after the nth component of the first m rows of $[Z]$ supplied by the user augment $[X]$.

zei a switch control concerning augmentation on the functions to be approximated. If $r=0$, this switch is ignored. With $zei=1$, regular augmentation is applied to the functions during the calculation. The n components of the first r rows of $[Y]$ supplied by user will be augmented by p zeros when moving $[Y]$ to $[X]$. With $zei=2$, special augmentation is applied. The first n components of the first r rows of $[Y]$ are the functional values supplied by user. The next p components of the first r rows of $[Y]$ are special values also supplied by user.

mui a switch control concerning weights. $[W]$ is an $n \times n$ real, positive definite, symmetric matrix of weights. It is generally diagonal and often the Identity matrix. $mui=1$ when $[W]=I_n$, the matrix $[W]$ need not be supplied. $mui=2$ when $[W]$ is diagonal, but not I_n. The procedure is supplied the n diagonal elements of $[W]$, but stored in the first row of matrix $[W]$. $mui=3$ when the full weighting matrix is supplied to the procedure.

The following list of matrix arrays is given to aid the user in determining the number of components and vectors in the input and results. $W[1{:}n,1{:}n]$, $Y[1{:}r,1{:}n+p]$, $Z[1{:}m,1{:}n+p]$, $X[1{:}m+1,1{:}n+p]$, $DEV[1{:}r,1{:}n]$, $COF[1{:}r,1{:}p]$, $STD[1{:}r]$, $CV[1{:}p+1,1{:}p]$, $VCV[1{:}r,1{:}p+1,1{:}p]$, $Q[1{:}r,1{:}m+1]$, $Q2$, E, $EP[1{:}r,1{:}m]$, $A[1{:}m,1{:}p]$, $GF[1{:}m+r]$, $ENF[1{:}m]$.

The results of the procedure are stored in the following locations. The user must be sufficiently familiar with the theory to know which results are relevant to his application of the procedure. All vectors are stored row-wise in the matrices listed below.

X orthonormal vectors
DEV deviations
COF coefficients
STD standard deviations
CV covariance matrix, stored in upper triangular form. The $(p+1)$st row contains the square root of the diagonal elements of the matrix.
VCV variance-covariance matrices, stored in upper triangular form with the $(p+1)$st rows containing the square root of the diagonal elements. There are r such matrices, the first subscript running over the r values.
gmdt Gram determinant value
Q Fourier coefficients
Q2 squared Fourier coefficients
E sum of the squared residuals
EP residuals
A a lower triangular matrix used to calculate the covariance matrix. $CV = A'A$.
GF Gram factors
ENF norms of the approximating vectors;

```
  begin
integer npp, npm, m1, n2, m2, r1, rbar, p2, bei, rhi, i18, gai, sii, i,
  j, dei, mui, elz1, elz2, k, thi, ali, omi, nii;
array PK,XP[1:n+p], QK[1:m+1];
real denom,sum,dk2,dk,fi,ss,ssq;
switch be := be1, be2; switch rh := rh1,rh2; switch ga :=
```

```
  ga1,ga2;
switch si := si1,si2; switch de := de1,de2; switch nu :=
  nu1,nu2;
switch th := th1,th2,th3; switch al := al1,al2;
switch om := om1,om2;
npp := n+p; npm := n+m; m1 := m-1; n2 := n+1; m2 := m+1;
r1 := 0; rbar := r; p2 := p+1; denom := if n=m then 1.0
else sqrt(n-m); bei := rhi := i18 := 1;
if (p≠0) then gai := sii := 2 else gai := sii := 1;
box1:  go to at[ai];
  at1: for j := 1 step 1 until n do begin
       X(2,j) := Z(1,j); X[1,j] := 1.0 end;
       for i := 2 step 1 until m1 do begin
       for j := 1 step 1 until n do
       X[i+1,j] := X[i,j] × X[2,j] end; go to box2;
  at2: for i := 1 step 1 until m do begin
       for j := 1 step 1 until n do
       X[i,j] := Z[i,j] end;
box2:  if p=0 then go to box3 else go to au[aui];
  au1: for i := 1 step 1 until m do begin
       for j := n2 step 1 until npp do
       X[i,j] := 0.0; X[i,n+i] := 1.0 end; go to box3;
  au2: for i := 1 step 1 until m do begin
       for j := n2 step 1 until npp do
       X[i,j] := Z[i,j] end;
box3:  dei := nui := e1z1 := e1z2 := k := 1;
box4:  thi := 1;
box5:  ali := omi := 1; if p=0 then go to box6 else
       for j := 1 step 1 until p do PK[n+j] := 0.0;
box6:  go to mu[mui];
  mu1: for i := 1 step 1 until n do PK[i] := X[k,i];
       go to box7;
  mu2: for i := 1 step 1 until n do
       PK[i] := X[k,i] × W[1,i]; go to box7;
  mu3: for i := 1 step 1 until n do begin sum := 0.0;
       for j := 1 step 1 until n do sum := sum + X[k,j] ×
       W[i,j]; PK[i] := sum end;
box7:  go to om[omi];
  om1: for i := 1 step 1 until k do begin sum := 0.0;
       for j := 1 step 1 until npp do
       sum := sum + PK[j] × X[i,j]; QK[i] := sum end;
       go to box8;
  om2: dk2 := 0.0; for i := 1 step 1 until npp do
       dk2 := dk2 + PK[i] × X[k,i];
       dk := sqrt(dk2);
       GF[i18] := dk; i18 := i18 + 1;
       for i := 1 step 1 until npp do
       X[k,i] := X[k,i]/dk;
       omi := 1; go to box6;
box8:  go to de[dei];
  de1: e1z1 := -e1z1; if e1z1<0 then go to box8b else
       go to box8a;
box8a: for i := 1 step 1 until k-1 do
       QK[i] := -QK[i]; QK[k] := 1.0;
       for i := 1 step 1 until npp do begin
       sum := 0.0; for j := 1 step 1 until k do
       sum := sum + X[j,i] × QK[j];
       XP[i] := sum end; go to box9;
box8b: ENF[i18] := sqrt (QK[k]); go to box8a;
  de2: e1z2 := -e1z2; if e1z2<0 then go to box8c else
       go to box8a;
box8c: for i := 1 step 1 until m do begin
       Q[r1,i] := QK[i]; Q2[r1,i] := QK[i] × QK[i] end;
       Q[r1,m2] := QK[m2]; E[r1,1] := Q[r1,m2]-Q2[r1,1];
       for j := 2 step 1 until m do
       E[r1,j] := E[r1,j-1] - Q2[r1,j];
       fi := 1.0;
       for i := 1 step 1 until m do begin
       if (fn-fi)>0.0 then begin if E[r1,i]<0.0 then begin
       EP[r1,i] := -sqrt(abs(E[r1,i])/(fn-fi)); go to box8d;
       end
       else EP[r1,i] := sqrt(E[r1,i]/(fn-fi));
       go to box8d; end else E[r1,i] := -1.0;
box8d: fi := fi+1.0; end go to box8a;
box9:  go to th[thi];
  th1: for i := 1 step 1 until npp do
       X[k,i] := XP[i]; go to box10;
  th2: for i := 1 step 1 until n do
       DEV[r1,i] := XP[i];
       for i := 1 step 1 until p do
       COF[r1,i] := -XP[n+i]; thi := 3; go to th1;
  th3: go to box11;
box10: go to al[ali];
  al1: omi := ali := 2; go to box6;
  al2: if k<m then begin k := k+1; go to box4; end
       else go to box12;
box11: go to nu[nui];
  nu1: nui := 2; go to box14;
  nu2: ss := dk/denom; ssq := ss × ss;
       STD[r1] := ss; go to box14;
box12: go to be[bei];
  be1: for i := 1 step 1 until m do begin
       for j := 1 step 1 until p do
       A[i, j] := X[i, n + j] end;
       gmdt := 1.0; for i := 1 step 1 until m do
       gmdt := gmdt × (GF[i]/ENF[i]);
       gmdt := gmdt × gmdt; dei := bei := thi := 2;
       k := k + 1; go to box13;
  be2: go to box11;
box13: go to ga[gai];
  ga1: go to box11;
  ga2: for i := 1 step 1 until p do begin
       for j := i step 1 until p do begin
       sum := 0.0;
       for nii := 1 step 1 until m do
       sum := sum + A[nii, i] × A[nii, j];
       CV[i, j] := sum end end;
       for i := 1 step 1 until p do
       CV[p2, i] := sqrt(CV[i, i]); gai := 1; go to box11;
box14: go to rh[rhi];
  rh1: if rbar = 0 then go to final else rbar := rbar -1;
       r1 := r1 + 1; thi := rhi := 2; go to ze[zei];
  ze1: for i := 1 step 1 until n do
       X[m2, i] := Y[r1, i];
       for i := 1 step 1 until p do
       X[m2, n+i] := 0.0; go to box5;
  ze2: for i := 1 step 1 until npp do
       X[m2, i] := Y[r1, i]; go to box5;
  rh2: go to si[sii];
  si1: go to rh1;
  si2: for i := 1 step 1 until p do begin
       for j := i step 1 until p do
       VCV[r1, i, j] := ssq × CV[i, j] end;
       for i := 1 step 1 until p do
       VCV[r1, p2, i] := ss × CV[p2, i]; go to rh1;
final: end ortho
```

CERTIFICATION OF ALGORITHM 127 [F5] ORTHO [Philip J. Walsh, *Comm. ACM 5* (Oct. 1962)]

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KEY WORD AND PHRASES: orthogonalization, approximation
CR CATEGORIES: 5.13, 5.17, 5.5

Algorithm 127 contains the following errors.

1. A **begin** must appear between the 6th and 7th lines, i.e. immediately after the integer specification and before the switch declaration. The **begin** following the **comment** and preceding the integer declaration must be removed.
2. In the second integer declaration the identifiers *mui*, *elz*1, *elz*2 should be *nui*, *e*1*z*1, *e*1*z*2, respectively.
3. The section of the statement labeled *at*1 that reads $X(2, j) := Z(1, j)$ should read $X[2, j] := Z[1, j]$.
4. Following the statement labeled *box*8*d* there should be a semicolon between **end** and **go to** *box*8*a*.
5. The formal parameter *fn* is not defined or mentioned in the comment. It appears in the program between the labels *box*8*c* and *box*8*d*. If *fn* is put equal to *n* the array *EP* then contains unbiased estimates of the *m* standard deviations.

We have not needed the generalized definition of an inner product [1, p. 348] but have often required n (number of components per vector) to be large. We thus replaced the array $W[1:n, 1:n]$ by an array $W[1:n]$ which necessitated the removal of the switch list element *mu*3 from the 8th line, also an alteration to the line before the statement labeled *mu*3 and the removal of the three lines beginning with the statement labelled *mu*3. Consequently that part of the program that appeared in the six lines beginning with the statement labeled *mu*2 and ending with the statement labeled *box*7 then read as follows:

```
mu2:  for i := 1 step 1 until n do
        PK[i] := X[k, i] × W[i];
      box7:  go to om[omi];
```

After the above modifications and corrections had been included the program ran successfully on an English Electric KDF9 computer using both the Whetstone ALGOL compiler and the Kidsgrove ALGOL compiler, these codes being proper subsets of ALGOL 60.

Some of the problems used in testing Algorithm 127 were from approximation theory as applied to boundary value problems of elliptic type. For one such problem linear approximating functions were used in which most of the coefficients of the best approximations are zero. The computed values of the standard deviations sometimes differed by more than 10 percent from both the true values and the unbiased estimates. We also solved the Dirichlet problem described by Davis [1, p. 369]. The set of coefficients obtained for the approximating function agreed only to the third decimal place with those given in [1]. All our calculations were in single-precision floating-point arithmetic.

Rice [2, p. 325] has recently noted that once the Gram-Schmidt orthogonalization method loses orthogonality it produces almost identical vectors. However, Algorithm 127 includes a correcting device which gives a second and better estimate to the true value of an orthonormal vector once the value obtained by Gram-Schmidt is known. Thus although Rice's modifications were included in the program we have not noticed any significant differences in computational behaviour.

REFERENCES:

1. DAVIS, P. J. *Orthonormalizing codes in numerical analysis.* In *Survey of Numerical Analysis*, J. Todd (Ed.), McGraw-Hill, New York, 1962, pp. 347–379.
2. RICE, J. R. Experiments on Gram-Schmidt orthogonalization. *Math. Comput. 20* (Apr. 1966), 325–328.

ALGORITHM 128
SUMMATION OF FOURIER SERIES

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```
procedure Fourier (X, r, w, n, A, B);
  value n; real X, w, A, B; integer r, n;
  comment Fourier sums a one-dimensional Fourier series,
    using a recurrence relation described by Watt [Computer
    J. 1, 4 (1959) 162]. The parameters are the coefficients X, which
    are selected by r, w, the argument and n the total number of
    terms in the series. On exit A = ∑(r=0 to n-1) X_r cos(rw) and
    B = ∑(r=0 to n-1) X_r sin(rw). Fourier is particularly efficient
    where X_r = 0 for all r > some r1 and X_r ≠ 0 for all r ≦ r1 .;
begin real t, tr, tr1, cosw2;
  tr1 := 0; cosw2 := 2 × cos(w);
  for r := n-1 step -1 until 0 do
  begin if X ≠ 0 then go to term end search for nonzero term;
  tr := 0; go to all zeroes;
term: tr := X; for r := r-1 step -1 until 0 do
  begin t := tr × cosw2 + X - tr1; tr1 := tr; tr := t end
    recurrence;
all zeros: A := tr - tr1 × cosw2/2; B := tr1 × sin(w)
end Fourier series
```

CERTIFICATION OF ALGORITHM 128 [C6]
SUMMATION OF FOURIER SERIES [M. Wells, *Comm. ACM 5* (Oct. 1962), 513]

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* Work supported by the U.S. Atomic Energy Commission

The body of *Fourier* was transcribed for the Dartmouth SCALP translator for the LGP-30 computer. After uniformizing the spelling of *zeros* (lines 5 and 9 in the procedure body), the program compiled and ran without difficulty.

In the procedure statement for *Fourier*, the actual parameter corresponding to X should be an expression depending on the actual parameter corresponding to r.

The SCALP program was tested for the finite series:

$$A = \sum_{r=0}^{n-1} \cos rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \cos(nw/2) + 1$$

$$B = \sum_{r=0}^{n-1} \sin rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \sin(nw/2)$$

for $w = 0.1, 0.2, 0.5$ and 1.0, and for $n = 1(1)51$. Although the algorithm appears to be numerically correct, the results showed evidence of serious numerical instability, particularly for small values of w. For $w = 0.1$, and $n = 51$, the error in A was .00109, and in B, $-.00231$. Since the largest A for $n < 51$ is 10.5, and the largest B about 20, the best result obtainable with the 7+ significant digit arithmetic of the SCALP system is about .00001. For comparison, a program summing the same series using a forward recurrence based on the addition formulas for the sine and cosine gave errors of .00012 and $-.00018$. It was, however, only about half as fast.

ALGORITHM 129
MINIFUN
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```
procedure MINIFUN (t1, b1, eps, n, ncnt, fmin, xmin, k1, GFUN);
  value t1, b1, eps, n, ncnt; integer n, ncnt, k1; real fmin;
  real procedure GFUN; array t1, b1, eps, xmin;
comment MINIFUN is a subroutine to find the minimum of a
  function of n variables, using the method of steepest descent.
  Input is:
  1. t1(i), i = 1,2, ··· , n, the upper limits of the search region
  2. b1(i), i = 1,2, ··· , n, the lower limits of the search region
  3. eps(i), i = 1,2, ··· , n, the convergence criteria. The func-
     tion must be a minimum in the region | x(i) − xmin(i) |
     ≦ eps(i)
  4. n, the number of variables (the dimension of the arrays)
  5. ncnt, the maximum number of iterations. The routine
     searches for a minimum until | x(i) − xmin(i) | ≦ eps(i)
     for all i, or until icnt = ncnt, whichever happens first.
  Output is:
  1. fmin, the minimum value of the function
  2. xmin(i), i = 1, ··· , n, the point at which the minimum
     occurs
  3. k1, an error code
     If k1 = 1, a minimum has been found within the specified
     number of iterations and the minimum is less than all
     values of the function at the centers of the planes forming
     the boundary of the epsilon-cube
     If k1 = 2, Δx(i) ≦ eps(i) but a new minimum has been found
     If k1 = 3, ncnt has been exceeded without Δx(i) ≦ eps(i).
     In this case, a test is made to see if the current minimum
     is a minimum in the epsilon-cube.
  MINIFUN has been written as a FORTRAN II subroutine and is
  available from the SMSA Computation Center. It should be
  noted that the FORTRAN II deck has been tested only on some
  relatively simple functions of two variables, such as GFUN
  (x,y) = cos(xy). The writer does not claim that the algorithm
  has been thoroughly tested;
begin integer j, i, icnt, k; real w, dmax, alamb, ft;
      array wnew [1:n], xt[1:n], x1b[1:n], xub [1:n],
        del x[1:n], d12x[1:n], xmin[1:n], x[1:n, 1:4], g[1:n, 1:4],
        dxmin[1:n], d2xmn[1:n];
  comment start looking for a minimum at midpoint of region;
  for j := 1 step 1 until n do
    begin wnew[j] := (t1[j] + b1[j])/2; xt[j] := wnew[j];
          xub[j] := t1[j]; x1b[j] := b1[j]; del x[j] := (xub[j]
            − x1b[j])/5;
          d12x[j] := del x[j]↑2; xmin[j] := xt[j]
    end;
  fmin := GFUN (xmin);
  for j := 1 step 1 until n do
    begin w := xt[j]; for i := 1 step 1 until 4 do
      begin x[j, i] := x1b[j] + i × del x[j];
            xt[j] := x[j,i]; g[j,i] := GFUN(xt);
      end;
      xt[j] := w;
      dxmin[j] := (g[j,3] − g[j,2])/del x[j];
      d2xmn[j] := (g[j,4] − g[j,3] − g[j,2] + g[j,1])/d12x[j]
    end;
  comment first and second difference quotients have been com-
          puted;
  icnt := 0; dmax := dxmin[1]; k := 1;
nustep: for j := 2 step 1 until n do
    begin if abs(dmax) < abs(dxmn[j]) then
          begin dmax := dxmin[j]; k := j
          end;
    end;
  alamb := dxmin[k]/d2xmn[k]; w := xt[k] − alamb;
comment a new coordinate has been computed for the variable
  having the largest first partial derivative. It will be checked to
  see if the new point still lies within the region and search will
  continue;
  if w < b1[k] then w := b1[k] else if w > t1[k] then w := t1[k];
  xt[k] := w; ft := GFUN(xt);
  if ft < fmin then go to check else
restart: if xt[k] < wnew[k] then go to 1bdchk
          else if xt[k] = wnew[k] then go to stnubds
          else if t1[k] > xt[k] then go to nupbds
          else xt[k] := 1.5 × wnew[k];
nupbds: xub[k] := t1[k]; x1b[k] := 2 × xt[k] − t1[k]; go to
  newdel;
stnubds: x1b[k] := xt[k] − 0.5 × wnew[k]; xub[k] := xt[k] +
  0.5 × wnew[k];
newdel: del x[k] := 0.2 × (xub[k] − x1b[k]); d12x[k] := del x[k]↑2;
    for i := 1 step 1 until 4 do
  begin x[k,i] := x1b[k] + i × del x[k]; w := xt[k];
        xt[k] := x[k,i]; g[k,i] := GFUN(xt); xt[k] := w
  end;
  dxmin[k] := (g[k,3] − g[k,2])/del x[k];
  d2xmn[k] := (g[k,4] − g[k,3] − g[k,2] + g[k,1])/d12x[k];
  icnt := icnt + 1;
  if icnt > ncnt then go to outcd else go to nustep;
1bdchk: if xt[k] ≦ b1[k] then xt[k] := 0.5 × wnew[k]
          else x1b[k] := b1[k]; xub[k] := 2.0 × xt[k] − b1[k];
    go to newdel;
check: fmin := ft; xmin[k] := xt[k];
  for j := 1 step 1 until n do if del x[j] > eps[j] then go to restart;
recheck: for j := 1 step 1 until n do
  begin w := xmin[j]; xmin[j] := w + eps[j]; ft := GFUN
        (xmin);
    if ft < fmin then go to set2; xmin[j] := w − eps[j];
    ft := GFUN(xmin); if ft < fmin then go to set2; xmin[j]
        := w
  end;
if k1 < 3 then k1 := 1; go to bgend;
set2: k1 := 2; go to bgend;
outcd: k1: =3; go to recheck;
bgend: end MINIFUN;
```

REMARK ON ALGORITHM 129 MINIFUN

MINIFUN [V. W. Whitley, *Comm. ACM*, Nov. 1962]

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Some errors found in Algorithm 129 *MINIFUN* [*Comm. ACM*, Nov. 1962] are given below.

In addition, the way "steepest descent" is used to compute the minimum of a function of n variables is not entirely satisfactory. The method for computing first derivatives may be improved in two ways:

1. Instead of computing $\frac{f(x+h)-f(x)}{h}$ it is better to take $\frac{f(x+h)-f(x-h)}{2h}$. As $f(x-h)$ has been computed by *MINIFUN* this does not give rise to extra computations.

2. In *MINIFUN* the choice of h seems rather deliberate. Indeed, h is taken as $.2 \times (xub-x1b)$, where xub and $x1b$ are variable bounds of x. In the beginning of the program these bounds are put equal to the fixed bounds $b1$ and ub; afterwards in the iteration process they should tend towards each other, and in the limit they provide the minimum. So especially when a good approximation to the minimum is unknown, $b1$ and ub have to be taken well apart from each other, which means that h is rather large. At the limit, however, h is very small. It is better to take h in such a way that the nominator $f(x+h)-f(x-h)$ attains an appropriate value.

As the method used by *MINIFUN* is the Newton-Raphson method applied to the first derivatives, convergence is not always secured—especially since first and second partial derivatives are estimated with numerical methods.

It should be noted that the test on end of program is not correct. For a further possible decrease of the function one has not to look in the direction of the coordinate axes but in the direction of the steepest descent.

ALGOL descriptions of some "steepest descent" programs which were written in the symbolic code of the Philips computer Pascal [cf. H. J. Heijn and J. C. Selman, *IRE Trans. EC10* (June 1961), 175–183] are given in Algorithms 203, 204 and 205.

CORRECTIONS OF *MINIFUN*:

Printing errors: The line below label *nustep* should read:

begin if *abs*(*dmax*) <*abs* (*dxmin* [*j*]) **then**

The label 1 *bdchk* should be *lbdchk*

In **comment** *MINIFUN*: *k*1=2: a new minimum has not been found.

The **label** nustep should be placed before the statement: *dmax* := *dxmin*[*j*]; The declaration of *xmin* should be removed from the blockhead of the procedure body. The 2-dimensional arrays *x*[1:*n*, 1:4] and *g*[1:*n*, 1:4] can be replaced by a **real** *x* and a 1-dimensional **array** *g*[1:4] respectively.

An improvement could be the insertion of the statement

*k*1 := 1;

just before the **label** nustep.

I am having considerable trouble with the obviously important part played by the **array** *wnew*, although it does not change after being set in the first statement of the program. Furthermore it seems to me that *wnew* plays a double rôle: first the component *wnew*[*k*] is the value of *xt*[*k*] before an iteration on *xt*[*k*]. But then one should insert another statement after **label** *nustep*: *wnew*[*k*] := *xt*[*k*]; Secondly *wnew*[*k*] is to be understood as half the distance between upper and lower bound *t*1[*k*] and *b*1[*k*], which is only true when *b*1[*k*] = 0.

Convergence of *de*1*x*[*j*] to 0 is only achieved when *x*1*b*[*k*] and *xub*[*k*] are tending towards each other. This indicates that *wnew*[*k*] should go to 0 too. (See statements after **label** *stnubds*.)

The following modifications could remove these objections (starting with the line above **label** *restart*):

```
          if ft < fmin then go to check else xt[k] := wnew[k];
restart:  if xt[k] < wnew[k] then go to lbdchk;
          if xt[k] = wnew[k] then go to stnubds;
          if xt[k] < t1[k] then go to nupbds;
          xt[k] := 0.5 × (wnew[k] + t1[k]);
nupbds:   xub[k] := t1[k]; x1b[k] := 2 × xt[k] − t1[k]; go to
            newde1;
stnubds:  x1b[k] := xt[k] − 0.5 × (wnew[k] − x1b[k]);
            xub[k] := xt[k] + 0.5 × (wnew[k] − x1b[k]); (etc.)
lbdchk:   if xt[k] = b1[k] then xt[k] := 0.5 × (wnew[k] + b1[k]);
            x1b[k] := b1[k]; xub[k] := 2 × xt[k] − b1[k]; go to
            newde1; (etc.)
```

ALGORITHM 130
PERMUTE
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```
procedure PERMUTE (A, n, x)
array A; integer n, x;
comment Each entry into PERMUTE generates the next per-
  mutation of the first n elements of A. If A is read as a number
  (A[1]A[2] ··· A[n]), each generation is larger than the last:
  n := 4, x := 1
    A[1]   1 1 1 8 8 8
    A[2]   1 8 8 1 1 8
    A[3]   8 1 8 1 8 1      Permutations = 4!/2!2!
    A[4]   8 8 1 8 1 1 end
  Identical elements in A reduce the number of permutations. The
  array should be ordered before the first call on PERMUTE.
  Integer x specifies the first elements whose order should be pre-
  served: n := 4, x := 3
    A[1]   1 1 1 4
    A[2]   2 2 4 1          Permutations = 4!/3!
    A[3]   3 4 2 2
    A[4]   4 3 3 3 end
  Before the first call on PERMUTE for a given array, first
  should be made true. If more is true, then PERMUTE was able
  to give another permutation;
begin array B[1:n]; integer f, i, k, m, p; real r; own real t;
  if first then t := A[x]; first := false;
  for i := 1 step 1 until n do B[i] := 0;
  for i := n step -1 until 2 do
    begin if A[i] > t∧A[i] > A[i - 1] then go to find; end;
  more := false; go to exit;
find: for k := n step -1 until i do
        begin if A[k] > t∧A[k] > A[i -1] then
          begin B[k] := A[k]; m := k; end; end;
      for k := n step -1 until i do
        begin if B[k] > 0 ∧B[k] < B[m] then
          begin B[m] := B[k]; f := k; end; end;
      r := A[i - 1]; A[i - 1] := B[m]; A[f] := r;
schell: p := i - 1; m := n - p;
        for m := m/2 - .4 while m > 0 do
          begin k := n - m;
          for f := p + 1 step 1 until k do
            begin i := f;
comp:       if A[i] > A[i + m] then
              begin r := A[i + m]; A[i + m] := A[i];
              A[i] := r; i := i - m;
              if i ≧ p + 1 then go to comp;
              end end end schell;
exit. end PERMUTE
```

REMARKS ON:

ALGORITHM 87 [G6]
PERMUTATION GENERATOR
[John R. Howell, *Comm. ACM 5* (Apr. 1962), 209]
ALGORITHM 102 [G6]
PERMUTATION IN LEXICOGRAPHICAL ORDER
[G. F. Schrak and M. Shimrat, *Comm. ACM 5* (June (1962), 346]
ALGORITHM 130 [G6]
PERMUTE
[Lt. B. C. Eaves, *Comm. ACM 5* (Nov. 1962), 551]
ALGORITHM 202 [G6]
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER
[Mok-Kong Shen, *Comm. ACM 6* (Sept. 1963), 517]

R. J. ORD-SMITH (Recd. 11 Nov. 1966, 28 Dec. 1966 and 17 Mar. 1967)
Computing Laboratory, University of Bradford, England

A comparison of the published algorithms which seek to generate successive permutations in lexicographic order shows that Algorithm 202 is the most efficient. Since, however, it is more than twice as slow as transposition Algorithm 115 [H. F. Trotter, Perm, *Comm. ACM 5* (Aug. 1962), 434], there appears to be room for improvement. Theoretically a "best" lexicographic algorithm should be about one and a half times slower than Algorithm 115. See Algorithm 308 [R. J. Ord-Smith, Generation of Permutations in Pseudo-Lexicographic Order, *Comm. ACM 10* (July 1967), 452] which is twice as fast as Algorithm 202.

ALGORITHM 87 is very slow.

ALGORITHM 102 shows a marked improvement.

ALGORITHM 130 does not appear to have been certified before. We find that, certainly for some forms of vector to be permuted, the algorithm can fail. The reason is as follows.

At execution of $A[f] := r$; on line prior to that labeled *schell*, f has not necessarily been assigned a value. f has a value if, and only if, the Boolean expression $B[k] > 0 \wedge B[k] < B[m]$ is **true** for at least one of the relevant values of k. In particular when matrix A is set up by $A[i] := i$; for each i the Boolean expression above is **false** on the first call.

ALGORITHM 202 is the best and fastest algorithm of the exicographic set so far published.

A collected comparison of these algorithms is given in Table I. t_n is the time for complete generation of $n!$ permutations. Times are scaled relative to t_8 for Algorithm 202, which is set at 100. Tests were made on an ICT 1905 computer. The actual time t_8 for Algorithm 202 on this machine *was* 100 seconds. r_n has the usual definition $r_n = t_n/(n \cdot t_{n-1})$.

TABLE I

Algorithm	t_6	t_7	t_8	r_6	r_7	r_8
87	118	—	—	—	—	—
102	2.1	15.5	135	1.03	1.08	1.1
130	—	—	—	—	—	—
202	1.7	12.4	100	1.00	1.00	1.00

ALGORITHM 131
COEFFICIENT DETERMINATION*

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* This procedure pertains to research work sponsored in part by NSF Grant G-7361.

```
procedure  DET (n, G, H);
array      G, H;  integer n;
comment    Given the first n coefficients of the power series
  G(z) = g1 + g2z + g3z^2 + ··· + gnz^(n-1) + ··· , and H(z) = h1 +
  h2z + h3z^2 + ··· + hnz^(n-1) + ··· , this procedure determines the
  coefficients di , i = 1, ··· , n, of the power series which is the
  expansion of the quotient H(z)/G(z). It is assumed that g1 ≠ 0.
  The arrays G and H initially contain the coefficients of G(z) and
  H(z), respectively. The integer n is the number of known coeffi-
  cients in the expansion of G(z) and H(z). At the conclusion, Hi
  contains the coefficient di . The procedure may also be useful in
  calculating residues for certain complex functions. Suppose
  F(z) = H(z)/G(z) is a complex valued function of a complex
  variable and that F has a pole of order m at z = b, where H(z) =
  Σ(k=1..∞) hk(z - b)^(k-1), G(z) = Σ(k=1..∞) gk(z - b)^(k+m-1), and g1 ≠ 0,
  h1 ≠ 0. The required residue at z = b is dm where

        D(z) = [ Σ(k=1..∞) hk(z - b)^(k-1) ] / [ Σ(k=1..∞) gk(z - b)^(k-1) ]

             = Σ(j=1..∞) dj(z - b)^(j-1).

  For more on this, one is referred to Einar Hille, "Analytic Func-
  tion Theory, Vol. I, " Ginn and Co., 1959, pages 242-244;
begin integer  i, j, n;  real alpha, beta;
               alpha := 1/G[1];
          for  j := 1 step 1 until n do
        begin  beta := alpha × H[j];
          for  i := j + 1 step 1 until n do
               H[i] := H[i] - (beta × G[i - j + 1]) end;
          for  j := 1 step 1 until n do
               H[j] := H[j] × alpha;
end            DET
```

ALGORITHM 132
QUANTUM MECHANICAL INTEGRALS OVER ALL SLATER-TYPE INTEGRALS

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```
real procedure: allslater (p,q,pe,qe,np,nq,lp,lq,mp,mq,na,nb)
                internuclear distance: (r);
                real pe,qe,r; integer p,q,np,nq,lp,lq,mp,mq,
                  na,nb;
comment The Slater-type orbitals frequently used in quantum
  mechanical calculations on atoms and molecules are defined as
  p = k(np,pe) r^(np-1) e^-(pe)r Y_lp^mp(θ, φ), where k(np,pe) is a normal-
  ization constant, Y_1^m(θ,φ) is a spherical harmonic with the
  phase convention [Y_1^m(θ,φ)]* = (-1)^m Y_1^-m(θ,φ), np is a positive
  integer, lp is an integer, lp < np, mp is an integer, - lp ≦ mp
  ≦ lp; and pe is a real positive constant. Algorithm 110, Y. A.
  Kruglyak and D. R. Whitman (Comm. ACM, July 1962) serves
  to compute integrals over certain operators of a quite restricted
  class of Slater-type orbitals, np ≧ 4, lp = 1, mp = 0. The algo-
  rithm given here will compute all integrals of the form
                        ∫ p_c(r_c^nc) q_c dr
  which can be expressed in terms of the simple A_n(b) and B_n(a)
  functions. The subscript c denotes either of the two nuclei of
  a diatomic molecule. These integrals include all those one-elec-
  tron integrals necessary for a conventional energy calculation
  on a diatomic molecule. In the arguments of allslater p and q
  are numerical designations for the respective orbitals. p and q
  are even or odd as they respectively are associated with the
  "left," a, nucleus or "right," b, nucleus of a diatomic molecule.
  Global arrays, fact 1, of factorials and binom, of binomial co-
  efficients are assumed. We first define some procedures utilized
  by allslater. The main program begins at the label set;
begin real norm, r2, alpha, beta, s, clp, clq, bpci;
  integer nsum, lsum, peven, qeven, podd, godd, limitp, limitq,
  g, h, i, j, n1p, n1q, lmp, lmq, gama, gamb, aidaa, aidab, gam,
  aida, num2; real array avalues [0:21], bvalues[0:21]; real pro-
  cedure c1, bpc, modulus;
real procedure c1(l,m,j); value l,m,j, integer l,m,j;
  begin c1 := ((-1)↑j)× fact1[2×(l - j)]/((2↑l) × fact1
    [l-2×j-m]×
    fact1[l - j]× fact1[j])
  end c1;
real procedure bpc(i, j, k); value i,j,k, integer i,j,k;
  begin real t; integer m; t := 0;
    for m := 0 step 1 until k do
    begin t := t + ((-1) ↑ (k - m)
      × binom [i, m] × binom [j, k - m]
    end
  end bpc;
real procedure modulus (i, j); value i, j; integer i, j;
  begin modulus := 1 -abs(i ÷ j) × j
  end modulus;
procedure avector (b, nmax, avalues); value b, nmax;
    real b; integer nmax; real array avalues;
  begin integer m;
    avalues[0] = exp(-b)/b;
    if nmax = 0 then go to exit;
    for m = 1 step 1 until nmax do
    begin avalues[m] = avalues[0] + (m/b) × avalues[m - 1]
    end;
exit: end avector;
procedure bvector(a nmax, bvalues); value a, nmax; real a;
  integer nmax; real array bvalues; real procedure modulus;
comment This procedure computes a sequence of values for the
  integral, B_n(a) = ∫_-1^1 x^n e^-ax dx, for n = 0 to n = nmax. If a ≧
  alim then B_0(a) is computed and upward recursion is used to
  generate the higher n values. If a < alim then B_nmax(a) is com-
  puted by series expansion and downward recursion is used to
  generate the smaller n values. alim is determined within the
  program by a simplification of a result of Gautschi (J. ACM 8,
  21 (1961)). Gautschi has made an analysis of the recursive pro-
  cedures for the B_n(a) which could be taken as a model for workers
  in molecular quantum mechanics;
  begin real fxx, fxy, numerator, denom, sum, factor1, tsum
    factor2, t, aa; integer m,mn;
    begin if abs(a) ≧ ((nmax+nmax/6+3)/2.3) then
      up: begin fxx := exp(a);
            fxy := 1/fxx;
            bvalues [0] := (fxx-fxy)/a;
            for m := 1 step 1 until nmax do
          begin fxx := - fxx;
            bvalues[m] := (fxx-fxy + m ×
            bvalues[m-1])/a
          end;
          go to exit;
        end up;
      down: begin aa := axa;
            if modulus (nmax, 2)≠0 then
          setodd: begin numerator := nmax + 2;
              sum := a/numerator;
              factor1 := -2;
              factor2 := 3;
              go to compute;
            end setodd;
          seteven: begin numerator := nmax + 1;
              sum := 1/numerator;
              factor1 := factor2 := 2;
            end seteven;
          compute: begin denom := numerator + 2;
              t := sum;
              t := ((((t/factor2)×aa)
                /(factor2-1))×numerator)
                /denom;
              tsum := t + sum;
              if (sum-tsum)=0 then
              begin bvalues[nmax] := sum × factor1;
                go to recur;
              end;
            begin factor2 := factor2 + 2;
                numerator := denom;
                sum := tsum;
              go to compute;
            end compute;
          recur: begin fxx := exp(a);
                fxy := 1/fxx;
                mn := nmax -1;
                if modulus(nmax, 2) ≠ 0 then
                fxx := -fxx;
                for m := mn step -1 until 0 do
                begin fxx = -fxx;
```

```
                        bvalues[m] := (fxx+fxy + a ×
                        bvalues[m+1])/(m+1);
                    end
                end recur;
            end down;
    end;
exit: end bvector;
set: begin if (mp + mq) ≠ 0 then
        begin allslater := 0.0; go to exit end;
     set: begin norm := sqrt (((2×pe)↑
          (2×np+1) × (2×lp+1) × fact1[lp−mp] × (2×qe)↑
          (2×nq+1) × (2×lq+1) × fact1[lq-mq])/(fact1[2×
          np] × fact1[lp+mp] × fact1[2×nq] × fact1[lq+mq] ×
          4));
          nsum := np+nq;
          lsum := lp+lq;
          r2 := r/2;
          norm := norm × (r2↑(nsum+1+na+nb));
          alpha := r2 ×(pe+qe);
          beta := r2 ×(((−1)↑p)×pe + ((−1)↑q) × qe);
          num2 := 2;
          avector (alpha, nsum, avalues);
          bvector (beta, nsum, bvalues);
          peven := modulus (p+1,2);
          qeven := modulus (q+1,2);
          podd := modulus (p,2);
          qodd := modulus (q,2);
          limitp := (lp−mp)÷num2;
          limitq := (lq−mq)÷num2;
          s := 0;
     end set;
sum: begin for g := 0 step 1 until limitp do
          begin c1p := c1(lp,mp,g);
          for h := 0 step 1 until limitq do
          begin c1q := c1(lq,mq,h);
          n1p := np−lp+2×g−1;
          n1p := nq−lq+2×h−1;
          lmp := lp−mp−2×g;
          lmp := lq−mq−2×h;
          gama := n1p × peven + n1q × qeven +1 +na;
          gamb := n1p × podd + n1q × godd +1 +nb;
          aidaa := lmp × peven + lmq × qeven;
          aidab := lmp × podd + lmq × qodd;
          gam = gama + gamb;
          aida = aidaa + aidab;
          for i := 0 step 1 until gam do
          begin bpci := bpc(gama, gamb, i);
          for j := 0 step 1 until aida do
          begin
          s := s+ c1p × c1q × bpci ×
          bpc(aidaa, aidab, j) ×
          avalues[nsum+na+nb−i−j]
          × bvalues[lsum −2 × (g+h) +i−j];
          end
          end
          end
          end;
      allslater := s × norm;
      end sum;
exit: end;
end allslater;
```

ALGORITHM 133
RANDOM

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```
real procedure RANDOM (A, B, X0);
value A, B, X0;
real A, B;
integer X0;
comment RANDOM generates a rectangular distributed
  pseudo-random number in the interval A < B. X0 is an integer
  starting-value. The first time RANDOM is used in a program
  X0 should be a positive odd integer with 11 digits, X0 < 2^35 =
  34 359 738 368. The following times RANDOM is used, X0 should
  be X0 = 0. The mathematical method used is X(n+1) = 5 Xn
  (mod 2^35). This sequence has period 2^33). RANDOM was suc-
  cessfully run on FACIT EDB using FACIT-ALGOL 1, which
  is a realization of ALGOL 60 for FACIT EDB, except for the
  declarator own, which is not included in FACIT-ALGOL 1.
  To test RANDOM, we computed 1/N Σ Xn and 1/N Σ Xn^2
  in the interval 0,1 for N = 500, 1000, 5000. The starting-
  value was X0 = 28 395 423 107. The results were 0.50625,
  0.48632, 0.50304 and 0.34304, 0.31681, 0.33469. Theoretically
  one expects 0.50000 and 0.33333;
begin
integer M35, M36, M37;
own integer X;
if X0 ≠ 0 then begin
X := X0; M35 := 34 359 738 368; M36 := 68 719 476 736;
M37 := 137 438 953 472 end; X := 5 × X;
if X ≧ M37 then X := X − M37;
if X ≧ M36 then X := X − M36;
if X ≧ M35 then X := X − M35;
RANDOM := X/M35 × (B − A) + A end
```

REMARK ON ALGORITHM 133
RANDOM (P. G. Behrenz, *Comm. ACM*, Nov. 1962)

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Replace the declarations in the body of the procedure,

integer *M35*, *M36*, *M37*; **own integer** *X*;

by:

own integer *X*, *M35*, *M36*, *M37*;

The sequence of 2^{33} random numbers contains about 15 numbers which are not really random numbers. For details, see R. W. Hamming, *Numerical Methods for Scientists and Engineers*, p. 384 [McGraw-Hill. 1962].

REMARK ON ALGORITHM 133
RANDOM [Peter G. Behrenz, *Comm. ACM 11*, Nov. 1962]

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Algorithm 133 was translated into FORTRAN II for the IBM 1620 and run successfully. The starting value was changed to 21 348 759 609 and significant results followed.

For $N = 500$ and 1000, the resulting values were: 0.4990157688, 0.4986269653 and 0.3318717863, 0.3290401482.

CERTIFICATION OF ALGORITHM 133
RANDOM [Peter G. Behrenz, *Comm. ACM*, Nov. 1962]

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Algorithm 133 was transliterated into FORTRAN II for the IBM 1620 computer. A monitor program performed the test indicated in Algorithm 133 on the generated numbers.

Results of the test are shown in the following chart. The notation used is identical to that used in the algorithm.

X_0	$\frac{1}{N}\Sigma X_n$	$\frac{1}{N}\Sigma X^2{}_n$	
	.4986480931	.3280561242	N = 500
13543288579	.4840396640	.3141520616	N = 1000
	.4996829627	.3321160892	N = 5000
	.4971414796	.3297990588	N = 500
24376589411	.4997720126	.3326801987	N = 1000
	.4986380784	.3319949173	N = 5000
	.4962408228	.3339214302	N = 500
34359738367	.4974837457	.3335720239	N = 1000
	.4929612237	.3253421270	N = 5000
	.5313808305	.3691599122	N = 500
11324679915	.5167083685	.3498558251	N = 1000
	.5043814637	.3383429327	N = 5000

ALGORITHM 134
EXPONENTIATION OF SERIES

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```
procedure SERIESPWR(A, B, P, N);
comment This procedure calculates the coefficients B[i] for
  the series (f(x))^P ≡ g(x) ≐ 1 + ∑ B[i] × x ↑ i, (i = 1, 2, ··· , N)
  given the coefficients of the series f(x) = 1 + ∑A[i] × x ↑ i.
  P may be any real number;
value A, P, N;
array A, B;
integer N;
begin integer i, k;
real p, s;
  B[1] := P × A[1];
  for i := 2 step 1 until N do
  begin s := 0;
    for k := 1 step 1 until i−1 do
    S := s + (P × [i−k] − k) × B[k] × A[i−k];
    B[i] := P × A[i] + (s/i)
    end for i;
  end SERIESPWR
```

CERTIFICATION OF ALGORITHMS 134 AND 158 EXPONENTIATION OF SERIES [Henry E. Fettis, COMM. ACM, Oct. 1962 and Mar. 1963]

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Work supported by the U.S. Atomic Energy Commission.

The bodies of SERIESPWR were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. In addition to the modifications required by the limitations of this translator, the following corrections were necessary:

1. Add "**real** P;" to the specifications.
2. Delete "p," from the declarations in the procedure body.
3. (134 only) Replace "S" by "s" and $[i-k]$ by "$(i-k)$" in the statement $S := s + \cdots$.
4. (158 only) Changes last sentence of comment to "Setting $P := 0$ gives the coefficients for $ln(f(x))$. In this series, the constant term is 0, instead of 1 as elsewhere;"
5. (158 only) Add the identifier $P2$ to the declared real variables.
6. (158 only) Make the first statements read:
   "**if** $P = 0$ **then** $P2 := 1$ **else** $P2 := P$;
   $B[1] := P2 \times A[1]$;
7. (158 only) Make the statement of the **for** k loop read

   "$S := S+(P\times(i-k)-k) \times B[k] \times A[i-k]$;"

8. Change the last statement to

   "$B[i] := P2 \times A[i] + S/i$ **end** for i;

In addition, the following modifications would improve the efficiency of the program:

1. Remove A from the value list.
2. Omit the statement $B[1] := P \times A[1]$; ($P2\times A[1]$ in 158 according to correction 6) and change the initial value of i in the statement following from 2 to 1.

When these changes were made, both procedures produced the first ten coefficients of the series for $(exp(x)) \uparrow 2.5$ from the first ten coefficients of the exponential series. The procedures were also used to generate the binomial coefficients by applying them to $(1+x)^P$, for $P = 2.0$, and 0.5000000. Algorithm 158 was also tested with $P := 0$ for $1+x$ and for the series expansions for $(sin\ x)/x$, $cos\ x$, and $exp\ x$. In all cases, the coefficients agreed with known values within roundoff.

ALGORITHM 135
CROUT WITH EQUILIBRATION AND ITERATION

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* This work was supported in part by the Office of Naval Research under contract Nonr 225(37).

```
procedure LINEARSYSTEM (A) order:(n) right-hand sides:(B)
  number of right-hand sides:(m) answers:(X) determinant:(det,
  ex) condition of A:(cnr);
integer n, m, ex; real det, cnr; real array A, B, X;
comment, LINEAR SYSTEM uses Crout's method with row
  equilibration, row interchanges and iterative improvement
  for solving the matrix equation AX = B where A is n × n and
  X and B are n × m. As special cases one sees that: for m ≦ 0,
  only the determinant of A is evaluated, for m = 1, the algo-
  rithm solves a system of n equations in n unknowns, for m = n
  and B = the identity matrix, the algorithm inverts A.
    If the algorithm breaks down for a singular or nearly singular
  matrix A, exit to a non-local label "singular" is provided. Five
  auxiliary procedures: EQUILIBRATE, CROUT, PRODUCT,
  RESIDUALS and SOLVE are declared with appropriate com-
  ments after the end of this procedure. This code is the result of
  the joint efforts of G. Guthrie, W. McKeeman, Cleve Moler,
  Margaret Salmon, Alan Shaw and R. Van Wyk. It was written
  following ideas presented by J. H. Wilkinson as a visiting lec-
  turer in Professor George E. Forsythe's class in Advanced Nu-
  merical Analysis at Stanford, 1962;
begin integer array pivot [1:n]; integer i, j, k; real mx;
  real array LU[1:n, 1:n], y, res, mult[1:n];
  comment, remove appropriate factors from the rows of A... ;
  EQUILIBRATE(A, n, mult);
  comment ... and save the result for the eventual computation
  of residuals during iteration;
  for i := 1 step 1 until n do
    for j := 1 step 1 until n do LU[i,j] := A[i,j];
  comment, decompose the matrix into triangular factors;
  CROUT(LU, n, pivot, det);
  comment, assuming that there was no exit to "singular",
  evaluate the determinant in the form det × (10.0 ↑ ex);
  for i := 1 step 1 until n do y[i] := LU[i,i] × mult[i];
  det := det × PRODUCT(y,1,n,ex);
  comment, now begin to process right-hand sides;
  for k := 1 step 1 until m do
  begin integer i, count, limit; real normy, kr;
    kr := k;
    comment, scale the right-hand side;
    for i := 1 step 1 until n do res[i] := B[i,k] := B[i,k]/mult[i];
    comment, store the first approximation and its L(1) norm;
    normy := 0;
    SOLVE(LU, n, res, pivot, y);
    for i := 1 step 1 until n do
    begin
      normy := normy + abs(y[i]);
      X[i,k] := y[i]
    end;
    comment, enter the iterating loop. The iteration is termi-
      nated on the integer "limit" which itself is determined on
      the basis of the success of the first iteration and a machine-
      dependent real number designated here by "eps". For
      "eps", the programmer must insert the largest real num-
      ber such that eps + 1.0 = 1.0 ;
    for count := 1, 2 step 1 until limit do
    begin integer i; real t;
      comment, compute the residuals of the solution y;
      RESIDUALS(A,n,B,k,X,res);
      comment ... and find the next increment to the solution;
      SOLVE(LU,n,res,pivot,y);
      comment, set up termination conditions;
      if count = 1 then
      begin real normdy;
        normdy := 0;
        for i := 1 step 1 until n do normdy := normdy+abs(y[i]);
        if normdy = 0 then begin cnr := 1.0; go to enditer end;
        t := normy/normdy;
        comment, The quantity ‖ A ‖·‖ A⁻¹ ‖ (spectral norm)
          is called the condition number of the matrix A. It is
          a measure of the difficulty in solving the input equation
          and appears naturally in error bounds for the solution
          (see Wilkinson [3]). cnr is a direct measure of the
          error and experimentally approximates the condition
          number;
        cnr := ((kr − 1.0) × cnr + 1.0/(eps × t))/kr;
        if t < 2.0 then go to singular;
        limit := ln(eps)/ln(1.0/t);
      end;
      comment, store the new approximation;
      for i := 1 step 1 until n do X[i,k] := X[i,k] := X[i,k]+y[i];
    end iteration;
    enditer:
  end right-hand sides
end LINEAR SYSTEM;
procedure EQUILIBRATE (A) order:(n) multipliers:(mult);
integer n; real array A, mult;
comment, scaling the rows of the matrix A to roughly the same
  maximum magnitude (here, dividing by the largest element)
  allows the procedure CROUT to select effective pivotal elements
  for the Gaussian decomposition of the matrix. The iterating
  procedure will converge to the solution for the equilibrated
  matrix rather than the input matrix. If the matrix is badly
  conditioned then the solution is sensitive to perturbations in
  the input and the scaling division must be done not by the
  largest element but rather by the power of the machine number
  base (2 and 10 for binary and decimal machines, respectively)
  nearest the largest element so as to avoid rounding errors.
  Equilibration is discussed in reference [3] p. 284;
begin integer i; real mx;
  for i := 1 step 1 until n do
  begin integer j;
    mx := 0.0; comment, find the largest element;
    for j := 1 step 1 until n do
      if abs(A[i,k]) > mx then mx := abs(A[i,k]);
    if mx = 0.0 then go to singular;
    comment, now store the multiplier and scale the row;
    mult[i] := mx; comment := base ↑ ex for exact scaling;
    if mx ≠ 1.0 then
      for j := 1 step 1 until n do A[i,j] := A[i,j]/mx
  end
end EQUILIBRATE;
```

```
procedure CROUT (A) order:(n) pivots:(pivot) interchanges:(sg).
integer n; integer array pivot; real array A; real sg;
comment, this is Crout's method with row interchanges as
  formulated in reference [1] for transforming the matrix A into
  the triangular decomposition LU with all the L[k,k] = 1.0.
  pivot[k] stores the index of the pivotal row at the k-th stage of
  the elimination for use in the procedure SOLVE;
begin integer i, j, k, imax, p; real t, quot;
 real procedure IP1 (A) extra term:(t) length:(f);
  integer f; real t; real array A; comment non-local i, j, k;
  comment, IP1 forms a row by column inner product of A,
    namely the sum of A[i,p] × A[p,k] for p := 1, 2, ... , f, and
    then adds the extra term t. If f < 1, the value of IP1 is t.
    This procedure is the inner loop of the algorithm. The pro-
    grammer can expect a substantial advantage from substi-
    tuting a faster and more accurate inner product here;
  begin real sum; integer p;
    sum := t;
    for p := 1 step 1 until f do sum := sum + A[i,p] × A[p,k];
    IP1 := sum
  end IP1;
  sg := 1.0;
  comment, k is the stage of the elimination;
  for k := 1 step 1 until n do
  begin
    t := 0;
    for i := k step 1 until n do
    begin comment, compute L. Note that the first calls on IP1
    are empty;
      A[i,k] := -IP1(A, -A[i,k],k-1);
      if abs(A[i,k]) > t then
        begin t := abs(A[i,k]); imax := i end
    end;
    if t = 0 then go to singular;
    comment, A[imax,k] is the largest element in the remainder
      of column k. Interchange rows if necessary and record the
      change;
    pivot[k] := imax;
    if imax ≠ k then
    begin
      sg := -sg;
      for j := 1 step 1 until n do
      begin
        t := A[k,j]; A[k,j] := A[imax, j]; A[imax, j] := t
      end
    end;
    comment, compute a column of multipliers;
    quot := 1.0/A[k,k];
    for i := k+1 step 1 until n do A[i,k] := A[i,k] × quot;
    comment, and compute a row of U;
    for j := k+1 step 1 until n do
      A[k,j] := -IP1(A,-A[k,j],k-1)
  end
end CROUT;
real procedure PRODUCT (factors) start:(s) finish:(f)
  exponent:(ex);
integer s,f,ex; real array factors;
comment, PRODUCT multiplies the numbers stored from index
  s through f inclusive in the array "factors", preventing ex-
  ponent overflow. The answer is normalized so that 1.0 > abs
  (PRODUCT) ≧ 0.1. The exponent appears in ex;
begin integer i; real p, p1;
  ex := 0; p := 1.0;
  for i := s step 1 until f do
  begin
    p1 := factors [i];
    if abs(p1) < 0.1 then begin p1 = 10.0 × p1; ex := ex-1
      end;
    p := p × p1;
    if p = 0 then begin ex := 0; go to fin end;
  1: if abs(p) < 0.1 then
    begin p := p × 10.0; ex : = ex-1; go to 1 end;
  2: if abs(p)≧1.0 then
    begin p := p/10.0; ex := ex + 1; go to 2 end;
  end;
  fin: PRODUCT := p
end PRODUCT;
procedure RESIDUALS (A) order:(n) right-hand sides:(B)
  column of B:(k) approximate solution:(X) residuals:(res);
  integer n, k; real array A, B, X, res;
comment, RESIDUALS computes b - Ay where b is the kth
  column of the right-hand side matrix B and y is the kth column
  of X;
    real procedure IP2 (A) row: (i) order:(n) approximate
      solution:(X)
    column:(k) extra therm:(t);
    integer i, k, n; real t real array A, X;
    comment, IP2 forms the inner product of row i of the matrix
      A and column k of the solution matrix X, then adds the
      single term t. It is essential that IP2 be an "accumulating"
      or double precision inner product as discussed in reference
      [3] p. 296. The value of IP2 is the rounded single precision
      result of the double precision arithmetic. The body of the
      procedure is left undefined;
begin integer i;
for i := 1 step 1 until n do
  res[i] := -IP2(A,i,n,X,k,-B[i,k])
end RESIDUALS;
procedure SOLVE (A) order:(n) right-hand side:(b) pivots:
  (pivot) answer:(y);
integer n; integer array pivot; real array A, b, y;
comment, SOLVE processes a right-hand side b and then back-
  solves for the solution y using the LU decomposition provided
  by CROUT;
begin integer k, p; real t;
  for k := 1 step 1 until n do
  begin
    t := b[pivot[k]]; b[pivot[k]] := b[k];
    for p := 1 step 1 until k-1 do t := t - A[k,p] × b[p];
    b[k] := t
  end ...having modified b by L inverse;
  comment, now the back solution for y;
  for k := n step -1 until 1 do
  begin
    t := b[k];
    for p := k+1 step 1 until n do t := t - A[k,p] × y[p];
    y[k] := t
  end backsolution
end SOLVE
```


REFERENCES

1. GEORGE E. FORSYTHE, Crout with Pivoting. Algorithm 16. *Comm. ACM 3*, 2 (Sept. 1960), 507.
2. DEREK JOHANN ROEK, Simultaneous System of Equations and Matrix Inversion Routine. Algorithm 92. *Comm. ACM 5*, 5 (May 1962), 286.
3. J. H. WILKINSON, Error Analysis of Direct Methods of Matrix Inversion, *J. ACM 8*, 3 (July 1961), 281-330.

CERTIFICATION OF ALGORITHM 135 CROUT WITH EQUILIBRATION AND ITERATION

[William Marshall McKeeman,* *Comm. ACM*, Nov. 1962]

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* This work was supported in part by the Office of Naval Research under contract Nonr 225(37).

A BALGOL translation of the algorithm was tested for accuracy, proper termination and running time on the Burroughs 220. The exact inverse of the Hilbert segment of order 6 can be stored in the 8-decimal-digit floating word of the B220 and was used in the accuracy and termination tests. The Hilbert segment H_6 is very ill-conditioned (for the spectral norm, $\| H_6 \| \cdot \| H_6^{-1} \| = 1.3 \times 10^7$). Hence the number of iterations required should not be taken as typical.

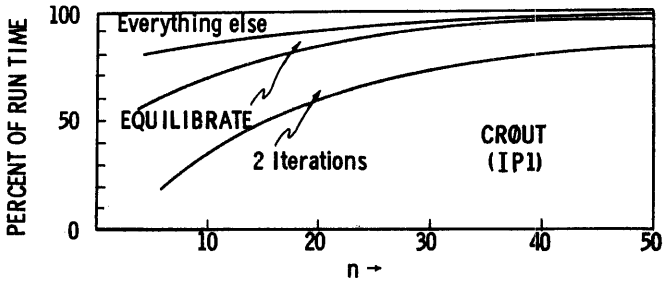
The $[n,n]$ element (mathematically $\frac{1}{11} = .090909 \cdots$) is representative of the behavior of the rest:

	"exact" equilibration (by powers of 10)	*equilibration by largest element in row*
initial solution	.092587535	.094091506
first iteration	.090877240	.091498265
second iteration	.090909695	.091570311
third iteration	.090909080	.091568310
fourth iteration	.090909091	.091568365
fifth iteration	terminated	.091568364
		terminated

Conclusions: The iterating procedure terminated correctly, or performed one extra iteration in each case. If the equilibration procedure alters the data, the iteration will converge to the solution for the altered matrix. If the matrix is ill-conditioned, as in the case above, the equilibration may cost a great deal more than it gains. As a practical matter, a machine language substitute for EQUILIBRATE which will not cause rounding of the data is probably the best course of action.

The running time is approximately proportional to n^3 as expected. If for a given machine, μ is the floating multiply time in seconds, one can expect that run time will be given by $rt := 1.3 \times \mu \times (n + 7) \uparrow 3$ seconds for a call on LINEARSYSTEM with one right-hand side.

The division of run time between the various phases of the algorithm is as follows:



REFERENCE:

1. SAVAGE AND LUKACS, Tables of inverses of finite segment of the Hilbert matrix. In Olga Taussky (Ed.), Contributions to the Solution of Systems of Linear Equations and the Determination of Eigenvalues, pp. 105–108, Nat. Bur. Standards Appl. Math. Series no. 39, U. S. Government Printing Office, Wash., D.C., 1954.

REMARK ON ALGORITHM 135 [F4] CROUT WITH EQUILIBRATION AND ITERATION

[W. M. McKeeman, *Comm. ACM 5* (Nov. 1962), 555–557, 559]

WILLIAM MARSHALL MCKEEMAN (Recd. 1 Apr. 1964)
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The following corrections to the published algorithm are recommended:

1. Two lines above the bottom line of procedure *SOLVE* one must change

$$y[k] := t \quad \text{to} \quad y[k] := t/A[k,k]$$

2. In procedure *EQUILIBRATE*, all occurrences of the subscript k must be changed to j.

3. The statement $cnr := 1.0$ should be added at the start of the body of procedure *LINEARSYSTEM*, so that *cnr* will have a value the first time it is used.

4. Line 19 from the end of *LINEARSYSTEM* should be changed from

if *normdy* = 0 **then begin** *cnr* := 1.0; **go to** *enditer* **end**;

to read

if *normdy* = 0 **then go to** *enditer*;

This correction makes sure that *cnr* retains a reasonable value in case *normdy* should be 0 for some column.

5. The symbol "-" must be removed from the parameter delimiters in the declarations of procedures *LINEARSYSTEM*, *RESIDUALS* and *SOLVE*.

6. Four lines above the bottom line of procedure *LINEARSYSTEM*, delete the first occurrence of $X[i,k] :=$

7. In the third line of the heading of procedure *IP2*, the parameter delimiter

) extra therm:(

should be changed to

) extra term:(

REMARK ON ALGORITHM 135 [F4] CROUT WITH EQUILIBRATION AND ITERATION

[W. M. McKeeman, *Comm. ACM 5* (Nov. 1962), 553–555, 557; *7* (July 1964), 421]

LOREN P. MEISSNER (Recd. 21 Oct. 1964)
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1. The following error in the published algorithm is noted: The procedure *IP*1 forms the sum of $A[i, p] \times A[p, k]$; however, two lines above the bottom line of procedure *CROUT* an attempt is made to use *IP*1 to form the sum of $A[k, p] \times A[p, j]$.

A possible way of correcting this is to add a procedure *IP*1*a* which is identical with *IP*1 except that k is written for i and j for k. Since the procedure is used often, making the correction in this way is not unreasonable. A more extensive undertaking would be to modify *CROUT* to use a more general procedure such as *INNERPRODUCT* [1].

2. The following comment is made in view of the reference to this algorithm in a recent Editor's Note [2]: In the use of Algorithm 135 as a determinant evaluator, it may be well to set m, the "number of right-hand sides" to 1 instead of zero and give an arbitrary nonzero right-hand side such as (1, 0, 0, ···). This will cause a calculation of the "condition," and possibly an exit to *singular*, to call the user's attention to cases in which the determinant is nonsense.

REFERENCES:
1. FORSYTHE, G. E. Crout with Pivoting. Algorithm 16. *Comm. ACM 3* (Sept. 1960), 507.
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ALGORITHM 136
ENLARGEMENT OF A GROUP
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* Currently with Burroughs Corporation, Pasadena, California

```
procedure Enlarge group (G, n, g, Abelian);
  array G, g; integer n; Boolean Abelian;
comment This procedure combines the element g with the sub-
  group G, of n elements, to form a new group. The Boolean
  Abelian has the value true if the group to which G and g belong
  is Abelian. Two procedures, multiply and equal are assumed
  to be declared: multiply (G[i]) by : (G[j]) to give : (G[k]) will set
  the element G_k equal to the product of the elements G_i and G_j.
  equal (G[i], G[j]) is a Boolean procedure whose value is true
  if, and only if, the elements G_i and G_j are equal. On leaving the
  procedure the enlarged group is in G, and n is equal to the
  number of elements in the new sub-group G. The procedure
  will function correctly if g is included in G on entry. It is prob-
  able that g and the elements of G will be arrays, and the pro-
  cedure body will, in practice, need to be altered considerably.
  The procedure has been used successfully in connection with
  problems of space-group theory;
begin integer i, j, k;
  for i := 1 step 1 until n do
  if equal (G[i], g) then go to not new generator;
  n := n + 1; G[n] := g;
  for i := n step 1 until n do
  begin for j := 1 step 1 until n do
  begin multiply (G[i], G[j], G[n+1]);
    for k := 1 step 1 until n do
    if equal (G[k], G[n+1]) then go to not new element 1;
    n := n + 1;
not new element 1: if Abelian then go to take next element;
  multiply (G[j], G[i], G[n+1]);
  for k := 1 step 1 until n do
  if equal (G[k], G[n+1]) then go to not new element 2;
  n := n + 1;
not new element 2: take next element:
  end of j-loop;
  end of i-loop;
not new generator: end of group enlargement
```

ALGORITHM 137
NESTING OF FOR STATEMENT I
DAVID M. DAHM & M. WELLS*
Burroughs Corp., Pasadena, Calif.
* On leave of absence from the University of Leeds, England.

```
procedure Fors 1 (n, P);
  value n; integer n; procedure P;
  comment Fors 1 generates a nest of n for statements with the
    procedure P at their center. Two non-local arrays I and U,
    which give the value of the controlled variable and its upper
    bound for each level are assumed to be declared;
  begin integer j;
    if n = 0 then P
    else for j := 1 step 1 until U[n] do
    begin I[n] :=j; Fors 1 (n-1,P) end end Fors 1
```

ALGORITHM 138
NESTING OF FOR STATEMENT II
DAVID M. DAHM & M. WELLS*
Burroughs Corp., Pasadena, Calif.
* On leave of absence from the University of Leeds, England.

```
procedure Fors 2 (P);
  procedure P;
  comment Fors 2 performs the same function as Fors 1, but is
    more economic of storage space. It is expected, however,
    that Fors 1 would be more economic of time. The formal
    parameter n is now replaced by the non-local integer n;
  begin if n = 0 then P
    else for I[n] := 1 step 1 until U[n] do
    begin n := n-1; Fors 2 (P) end;
    n := n + 1 end Fors 2
```

ALGORITHM 139
SOLUTIONS OF THE DIOPHANTINE EQUATION

J. E. L. PECK
University of Alberta, Calgary, Alberta, Canada

```
procedure Diophantus (a,b,c); integer a,b,c;
comment This procedure seeks the integer solutions of the
  equation ax + by = c, where the integers a,b,c are given. It
  assumes a non-local integer M, which should be as large as
  storage will allow, two nonlocal labels INDETERMINATE
  and NO SOLUTION and two non-local Boolean variables
  'general solution' and 'time permits' which are self explanatory.
  It also assumes the procedures abs, sign and print;
begin integer n,r,s,d,i; integer array q[1:M];
n := i := 0; d := s := abs(a); r := abs(b);
comment d will become the greatest common divisor of a and b.
  If b = 0 then d = | a |. The vector q will retain the successive
  quotients in the Euclidean algorithm r_{i-1} = r_i q_i + r_{i+1},
  i = 1, 2, ··· , n, where 0 ≦ r_{i+1} < r_i , r_0 = | a |, r_1 = | b |,
  and r_{n+1} = 0;
for i := i + 1 while r ≠ 0 do
  begin n := i; d := r; q[i] := s ÷ d;
  r := s - d × q[i]; s := d end This records the quotients and
    the number n of divisions for use below;
if d = 0 then go to if c = 0 then INDETERMINATE
else NO SOLUTION; comment The case d = 0 occurs when
  a² + b² = 0. If d now does not divide c then the equation can-
  not be solved so;
if (c ÷ d) × d ≠ c then go to NO SOLUTION;
if d ≠ 1 then
  begin a := a/d, b := b/d; c := c/d end, which removes
    the common factor and reduces the equation to the case
    where a and b are relatively prime;
  begin comment We shall now find u_1 and v_1 in order to
    express
    1 = au_1 + bv_1 , using the relations r_n = r_i v_i + r_{i-1} u_i ,
    i = n, n-1, ··· , 1, v_n = 1, u_n = 0, and r_{i+1} = -r_i q_i + r_{i-1} ,
    i = n-1, n-2, ··· , 1; integer u,v;
  if n = 0 then
    begin v := 0; u := 1 end, which takes care of the case
      b = 0
  else
    begin v := 1; u := 0;
    for i := n-1 step -1 until 1 do
      begin integer t;
      t := v; v := u - v × q[i]; u := t
      end i
    end the case n ≠ 0. It remains now to multiply the equality
      1 = au_1 + bv_1 through by c;
    begin integer x0, y0;
    x0 := c × u × sign(a); y0 := c × v × sign(b); print (x0,y0);
    comment If x_0 ,y_0 is a particular solution then x_0 ± ib,
      y_0 ∓ ia, i=1,2, ... gives the general solution. Therefore;
    if general solution then
      begin u := b; v := a;
      A: print(x0 + u, y0 - v); print(x0-u, y0 + v);
      u := u + b; v := v + a;
      if time permits then go to A
      end general solution and
    end solution.
end u,v
end Diophantus.
```

CERTIFICATION OF ALGORITHM 139 [A1]
SOLUTIONS OF THE DIOPHANTINE EQUATION

[J.E.L. Peck, *Comm. ACM 5* (Nov. 1962), 556]

HENRY J. BOWLDEN (Recd. 30 Sept. 1964 and 5 Nov. 1964)
Westinghouse Electric Corp., R&D Ctr., Pittsburgh, Pa.

Algorithm 139 was transcribed into Burroughs Extended ALGOL after the following typographical error was corrected: On the line following "**if** $d \neq 1$ **then**" replace "$a := a/d$," by "$a := a/d$;".

The cases shown in the table were tried, with the results shown in columns 4 and 5. These solutions are correct, but perhaps not too useful. Of course, a definition of "useful" in this context would be rather subjective; in any case, the user can always obtain an arbitrary solution "useful" for his purpose. We have chosen to regard a small value of x as a criterion for usefulness, and obtain this by inserting, just before "*print* (x0, y0)", the statements

$c := x0 \div b;\ x0 := x0 - c \times b;\ y0 := y0 + c \times a;$

The following remarks have to do with matters of programming taste rather than accuracy.

(a) A **value** part of form **value** *a, b, c*; should be inserted to avoid side effects.

(b) The results should be passed back to the calling program for use by the caller. This requires the addition of two call-by-name parameters (x0, y0), and the removal of the declaration **integer** x0, y0;. The provisions for printing the results should be omitted.

(c) The procedure contains a deliberate possibility of an infinite loop. This is unacceptable on most operating systems and should be omitted.

(d) The provision of an array (*q*) "as large as storage will allow" is rather indefinite. The algorithm as given provides no test to prevent exceeding this arbitrary size. The number of partial quotients in the Euclidean algorithm may be shown to be no more than five times the number of decimal digits in the (largest of the) coefficients *a, b, c*, so a size of five times the number of digits in the largest integer to be considered is sufficient.

The algorithm, modified as suggested above, gives the results in columns 6 and 7 of the table below. The execution time on the B-5000 was approximately 40 milliseconds.

			original		*modified*	
a	*b*	*c*	*x0*	*y0*	*x0*	*y0*
1000	23	1046	−2092	91002	−22	1002
0	0	0	indeterminate			
57	−103	47009	2209423	1222234	73	−416
10	12	578	−289	289	−1	49
10	12	97	no solution			

ALGORITHM 140
MATRIX INVERSION

P. Z. INGERMAN
University of Pennsylvania, Philadelphia, Penn.

```
procedure invert (a) of order:(n) with tolerance:(eps) and
  error exit:(oops);
value n, eps; array a; integer n; real eps; label oops;
comment This procedure inverts a matrix by using elementary
  row operations. Although the method is not particularly good
  for ill-conditioned matrices, the simplicity of the algorithm
  and the fact that the inversion occurs in place make it useful
  on occasion;
begin integer i;
  for i := 1 step 1 until n do
  begin integer j, k;  real q;
    q := a[i,i];
    if abs(q)≦abs(eps) then go to oops;
    a[i,i] := 1;
    if q≠1 then for k := 1 step 1 until n do a[i,k] := a[i,k]/q;
    for j := 1 step 1 until n do
      if i≠j then
        begin q := a[j,i];  a[j,i] := 0;
          for k := 1 step 1 until n do
            a[j,k] := a[j,k]-q×a[i,k] end end end
```

CERTIFICATION OF ALGORITHM 140
MATRIX INVERSION [P. Z. Ingerman, *Comm. ACM*, Nov. 1962]

RICHARD GEORGE*
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* Work supported by the United States Atomic Energy Commission.

Algorithm 140 was tested on the LGP-30, using SCALP, a load-and-go compiler from the Dartmouth College Computation Center, and it was shown to be syntactically correct.

It is indeed a simple procedure. It is so simple because the author has eliminated the very necessary search for largest elements and the row interchanges. As a result, this procedure will fail to invert many non-singular matrices. To be invertable by this procedure, a matrix must be such that all of its leading diagonal submatrices will have non-zero determinants.

One would do well to avoid this algorithm and use one (such as 120) which employs the pivoting process.

ALGORITHM 141
PATH MATRIX
P. Z. INGERMAN
University of Pennsylvania, Philadelphia, Penn.

```
procedure find path (a, n);
value n; Boolean array a; integer n;
comment This procedure is merely an Algol implementation
  of the method of Warshall (JACM 9(1962), 11-12). Some ad-
  vantage is taken of the characteristics of the problem to in-
  crease the efficiency;
begin integer i, j, k;
  for j := 1 step 1 until n do
  for i := 1 step 1 until n do
  if a[i,j] ∧ i≠j then
  for k := 1 step 1 until n do
  a[i,k] := a[i,k]∨a[j,k] end findpath
```

ALGORITHM 142
TRIANGULAR REGRESSION

W. L. HAFLEY AND J. S. LEWIS
Aluminum Company of America, Pittsburgh, Penn.

```
procedure trireg (n, nob, dep, pmax);
  real pmax; integer n, nob, dep;
  comment trireg is a multiple regression procedure which
    develops and inverts only the upper triangular portion of a
    correlation matrix of order n. The i,jth (i≦j) matrix element
    is r(ci+j) where the c's are cram numbers (ref. Algorithm 67,
    J. Caffey, Comm. ACM 4, July 1961). dep < n dependent
    variables are regressed simultaneously. Read (u) is an input
    procedure for single elements. The input consists of nob ob-
    servations on n variables. The first dep variables are con-
    sidered dependent and the remaining n − dep are considered
    independent variables. Independent variables are dropped
    when the pivotal element exceeds pmax during the inversion.
    Total variable storage is 14 + 3n + n(n+1)/2;
begin integer i1, i2, i3, c1, c2, c3, df; integer array c[1:n];
  real d, p, a; real array r[1:n(n+1)/2], v[1:n], m[1:n];
initial: df := 0; for i1 := 1 step 1 until n do m[i1] := 0;
         for i1 := 1 step 1 until n(n+1)/2 do r[i1] := 0;
input:   for i1 := 1 step 1 until nob do
         begin for i2 := 1 step 1 until n do Read (v[i2]);
           c1 := 0; for i2 := 1 step 1 until n do
             begin d := v[i2]; m[i2] := m[i2] + d;
               for i3 := i2 step 1 until n do
               begin c1 := c1 + 1; r[c1] := r[c1] + v[i3] × d end
             end i2;
         end i1;
correlation: c1 := 1; a := 1/nob; for i1 := 1 step 1 until n do
             begin v[i1] := 1/sqrt(r[c1]−(m[i1]↑2)×a);
               r[c1] := 1; c1 := c1 + n − i1
             end i1;
             c1 := 1; for i1 := 1 step 1 until n do
             begin d := a × m[i1]; p := v[i1]; c1 := c1 + 1;
               m[i1] := d;
               for i2 := i1 + 1 step 1 until n do
               begin r[c1] := (r[c1]−d×m[i2]) × v[i2] × p;
               end i2;
             end i1;
             comment variable i may be dropped from the
               regression by setting vi = 0 and df equal to the
               number of variables dropped;
cram:  i1 := − n; i2 := n + 1; for i3 := 1 step 1 until n do
         begin i1 := i1 + i2 − i3; c[i3] := i1
         end i1;
inversion: for i1 := dep + 1 step 1 until n do
           begin c1 := c[i1]; if v[i1] ≠ 0 then
             begin p := 1/r[c1+i1]; if p > pmax then
             begin df := df + 1; go to YY end else
               begin r[c1+i1] := p; for i2 := 1 step 1
                   until i1 − 1 do
                 begin c2 := c[i2]; a := p × r[c2+i1];
                   for i3 := i2 step 1 until n while i3 ≠ i1 do
                     begin if i3 < i1 then
                       begin c3 := c[i3]; d := r[c3+i1] end
                         else d := −r[c1+i3];
                       r[c2+i3] := r[c2+i3] + d × a
                     end i3;
                   end i2;
                   for i2 := i1 + 1 step 1 until n do
                   begin a := p × r[c1+i2]; c2 := c[i2];
                     for i3 := i2 step 1 until n do
                     r[c2+i3] := r[c2+i3] − a × r[c1+i3];
                   end i2;
                 ZZ: for i2 := 1 step 1 until i1 − 1 do
                   begin c2 := c[i2+i1]; r[c2] := − p × r[c2]
                   end i2;
                   for i2 := c1 + i1 + 1 step 1 until n + c1 do
                   r[i2] := p × r[i2]
                 end
               end else
             YY: begin p := 0; r[c1+i1] := 0; go to ZZ end
coeff:   d := 1/(nob−n+dep−l+df); for il := 1 step 1 until
           dep do
         if v[i1] ≠ 0 then
         begin a := 0; p := 1/v[i1]; c1 := c[i1]; for i2 := dep
           +1 step 1 until n do
           begin if r[i2] ≠ 0 then
             begin r[c1+i2] := −r[c1+i2] × v[i2] × p; a :=
               a + r[c1+i2] × m[i2]
             end
           end i2;
           v[i1] := (2−r[c1+i1]) × d/(v[i1]↑2)
           comment: v[1:dep] now contains the mean square
             deviations from regressions for the dependent vari-
             ables. The coefficients of determination R² may be
             obtained as r[c1+i1] − 1;
           r[c1+i1] := m[i1] − a else
           begin c1 := c[i1]; for i2 := c1 + i1 step 1 until
             c1 + n do r[i2] := 0
           end
         end
comment The r-array now contains the constants and coeffi-
  cients of regression, and the inverse of the correlation matrix of
  the independent variables that have been kept. The following
  example will help to locate the information in the r array.
  Example: n = 6 dep = 3

   r1 r2 r3 | r4  r5  r6      b01          | b11 b21 b31
      r7 r8 | r9  r10 r11         b02       | b12 b22 b32
         r12| r13 r14 r15            b03    | b13 b23 b33
            | r16 r17 r18                   | r11 r12 r13
               r19 r20                        r22 r23
                   r21                        r33

  The variances and covariances of the regression coefficients for
  the jth dependent variable can be determined by—
        Var (bij) = rii × vj × vi²
        Covar (bij bkj) = rik × vj × vi × vk;
end trireg
```

ALGORITHM 143
TREESORT 1
ARTHUR F. KAUPE, JR.
Westinghouse Electric Corp., Pittsburgh, Penn.

```
procedure TREESORT 1 (UNSORTED, n, SORTED, k);
  value n, k;
integer n, k; array UNSORTED, SORTED;
comment TREESORT 1 is a revision of TREESORT (ALGORITHM 113) which requires neither the "packed" array m
  nor the machine procedures pack, left half, right half, and minimum. The identifier infinity is used as nonlocal real variable
  with value greater than any element of UNSORTED;
begin integer i, j; array m1 [1:2×n−1];
  integer array m2 [1:2×n−1];
procedure minimum; if m1 [2×i] ≦ m1[2×i+1] then
  begin m1[i] := m1[2×i]; m2[i] := m2[2×i] end else
  begin m1[i] := m1[2×i+1]; m2[i] := m2[2×i+1] end minimum;
for i := n step 1 until 2 × n − 1 do begin m1[i] := UNSORTED
  [i−n+1]; m2[i] := i end
for i := n − 1 step −1 until 1 do minimum;
for j := 1 step 1 until k do
  begin SORTED [j] := m1[1]; i := m2[1]; m1[i] := infinity;
    for i := i ÷ 2 while i > 0 do minimum end
end TREESORT 1
```

ALGORITHM 144
TREESORT 2
ARTHUR F. KAUPE, JR.
Westinghouse Electric Corp., Pittsburgh, Penn.

```
procedure TREESORT 2 (UNSORTED, n, SORTED, k, ordered);
  value n, k;
integer n, k; array UNSORTED, SORTED; Boolean procedure ordered;
comment TREESORT 2 is a generalized version of TREESORT 1. The Boolean procedure ordered is to have two real arguments. The array SORTED will have the property that ordered (SORTED[i], SORTED[j]) is true when j > i if ordered is a linear order relation;
begin integer i, j; array m1 [1:2×n−1]; integer array m2 [1:2×n−1];
procedure minimum; if ordered (m1[2×i], m1[2×i+1]) then
  begin m1[i] := m1[2×i]; m2[i] := m2[2×i] end else
  begin m1[i] := m1[2×i+1]; m2[i] := m2[2×i+1] end minimum;
for i := n step 1 until 2 × n − 1 do begin m1[i] := UNSORTED [i−n+1]; m2[i] := i end
for i := n − 1 step −1 until 1 do minimum;
for j := 1 step 1 until k do
  begin SORTED[j] := m1[1]; i := m2[1]; m1[i] := infinity;
    for i := i ÷ 2 while i > 0 do minimum end
end TREESORT 2
```

ALGORITHM 145
ADAPTIVE NUMERICAL INTEGRATION BY SIMPSON'S RULE

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* This work was supported in part by the Office of Naval Research under contract Non4 225(37).

```
real procedure Integral (F) limits: (a, b) tolerance: (eps);
real procedure F; real a, b, eps;
begin comment Integral will numerically approximate the
    integral of the function F between the limits a and b by the
    application of a modified Simpson's rule. Although eps is a
    measure of the relative error of the result, the actual error
    may be very much larger (e.g. whenever the answer is small
    because a positive area cancelled a negative area). The pro-
    cedure attempts to minimize the number of function evalua-
    tions by using small subdivisions of the interval only where
    required for the given tolerance;
  integer level;
  real procedure Simpson (F, a, da, Fa, Fm, Fb, absarea,est,eps);
  real procedure F; real a, da, Fa, Fm, Fb, absarea, est, eps;
  begin comment Recursive Simpson's rule;
    real dx, x1, x2, est1, est2, est3, F1, F2, F3, F4, sum;
    dx := da/3.0; x1 := a + dx; x2 := x1 + dx;
    F1 := 4.0 × F(a+dx/2.0); F2 := F(x1);
    F3 := F(x2); F4 := 4.0 × F(a+2.5×dx);
    est1 := (Fa+F1+F2) × dx/6.0;
    est2 := (F2+Fm+F3) × dx/6.0;
    est3 := (F3+F4+Fb) × dx/6.0;
    absarea := absarea-abs(est) + abs(est1) + abs(est2) + abs(est3);
    sum := est1 + est2 + est3;
    level := level + 1;
    Simpson := if (abs(est-sum) ≦ eps × absarea ∧ est ≠ 1.0) ∨
        level ≧ 7 then sum
        else Simpson (F, a, dx, Fa, F1, F2, absarea, est1, eps/3.0)
          + Simpson (F, x1, dx, F2, Fm, F3, absarea, est2, eps/3.0)
          + Simpson (F, x2, dx, F3, F4, Fb, absarea, est3, eps/3.0);
    level := level −1;
end Simpson;
level := 1;
Integral := Simpson (F, b-a, F(a), 4.0 × F((a+b)/2.0), F(b),
          1.0, 1.0, eps)
end Integral 13
```

CERTIFICATION OF ALGORITHM 145
ADAPTIVE NUMERICAL INTEGRATION BY SIMPSON'S RULE [W. McKeeman. *Comm. ACM*, Dec. 1962]

WM. M. MCKEEMAN
Stanford University, Stanford, Calif.

Suggested changes in the code:

1. Replace all occurrences of *eps*/3.0 by *eps*/1.7.
2. Replace level ≧ 7 by level ≧ 20.
3. The second parameter *a* in the final call of Simpson was omitted; insert it.

With the above changes, a BALGOL translation of *Integral* has been tested successfully on a large number of functions. An example of its behavior is given below:

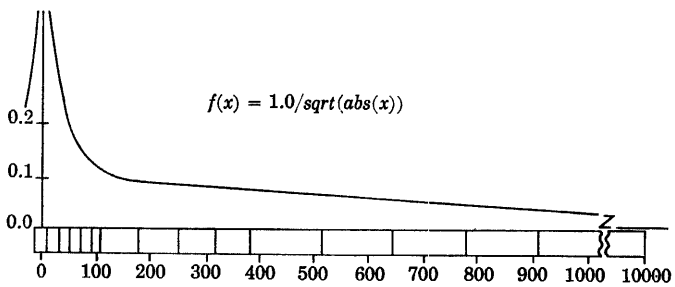
Machine: Burroughs 220, 8 decimal digit floating-point mantissa.
$f(x) = 1.0/sqrt(abs(x))$; which has a pole at the origin.
$a = -9.0$; $b = 1000.0$; correct answer = 206.0;

eps	computer answer	relative error
0.1	200.22251	0.028
0.01	206.00226	0.0000107
0.001	206.00092	0.0000045
0.0001	205.99985	0.0000007

If the recursion was allowed to go thirty levels deep we found:

0.0001 206.00005 0.0000002

The graph below shows the adaptive clustering of the points of evaluation around the pole of the function (taken from the first example above).



Each vertical line represents a point of evaluation for the function during the execution of the call:
integral(*f*, −9.0, 10000.0, 0.1);

REMARK ON ALGORITHM 145 [D1]
ADAPTIVE NUMERICAL INTEGRATION BY SIMPSON'S RULE [William Marshall McKeeman, *Comm. ACM 6*, (Dec. 1962), 604]

M. C. PIKE (Recd. 5 Oct. 1964 and 23 Nov. 1964)
Statistical Research Unit of the British Medical Research Council, University College Hospital Medical School, London, United Kingdom

This procedure was tested on the ICT Atlas computer and found satisfactory after the following three modifications were made:

(1) add "**real** *absarea*;" on the line following "**integer** *level*;",
(2) add "*absarea* := 1.0;" on the line following "*level* := 1;",
(3) substitute

"*Integral* := *Simpson* (*F*, *a*, *b*−*a*, *F*(*a*), 4.0×*F*((*a*+*b*)/2.0), *F*(*b*), *absarea*, 1.0, *eps*)"

for

"*Integral* := *Simpson* (*F*, *b*−*a*, *F*(*a*), 4.0×*F*((*a*+*b*)/2.0), *F*(*b*), 1.0, 1.0, *eps*)".

These corrections are necessary since *absarea* appears on the left-hand side of an assignment statement, namely, in line 10 of the **real procedure** *Simpson*, and yet when *Simpson* is called in the third to last line of the **real procedure** *Integral* the actual parameter for *absarea* is given as 1.0.

The author wishes to thank the referee for helpful suggestions.

ALGORITHM 146
MULTIPLE INTEGRATION

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* This work was supported in part by the Office of Naval Research under contract Non4 225(37).

```
real procedure MultipleIntegral (F) limits: (a, b) order: (n)
  tolerance: (eps);
real procedure F; real array a, b; real eps; integer n;
begin comment F is a function of n variables which are stored
    in an internal array x. MultipleIntegral approximates the
    multiple integral of F between the n pairs of limits stored in
    the parameter arrays a and b. For a mesh of k steps on each
    axis, the number of function evaluations required for an
    integral of nth order is approximately k↑n. One consequence
    is that the practical limit on n is quite small. Another is that
    any inefficiency in the (undefined) procedure Integral will
    reflect itself to the nth power in MultipleIntegral. The adap-
    tive procedure Integral is recommended;
  real array x[1:n+1]; integer axis;
  real procedure Integral (F) limits: (a, b) tolerance: (eps);
  real procedure F; real a, b, eps;
  begin comment The body of procedure Integral is left
    undefined. For it one may substitute any procedure of the
    same name that evaluates the integral of a function of a single
    variable between the real limits a and b;
  end Integral;
  real procedure MI(y); real y;
  begin comment Recursive multiple integration;
    x[axis] := y;
    axis := axis -1;
    MI := if axis = 0 then F(x) else
      Integral (MI, a[axis], b[axis], eps/n);
    axis := axis +1;
  end MI;
  axis := n + 1;
  MultipleIntegral := MI(0)
end MultipleIntegral
```

CERTIFICATION OF ALGORITHM 146
MULTIPLE INTEGRATION [W. M. McKeeman, *Comm. ACM 5* (Dec. 1962), 604]

NIKLAUS WIRTH (Recd. 6 Jan. 1964)
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Algorithm 146 was translated into a generalized ALGOL [cf. N. Wirth, A generalization of ALGOL, *Comm. ACM 6* (Sept. 1963), 547–554] and successfully run on the Stanford IBM 7090 computer. Algorithm 60, Romberg Integration [*Comm. ACM 4* (June 1961), 255; *5* (Mar. 1962), 168; *5* (May 1962), 281] was used for the real procedure *Integral*.

The main disadvantage of Algorithm 146 is that the bounds of the domain of integration must be constant, i.e. the domain must always have the form of a rectangular hyperbox.

ALGORITHM 147
PSIF

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Ministry of Defense, Israel

```
real procedure psif(x, a, tan, ln) exit: (errexit);
value x, a; label errexit; real procedure tan, ln;
comment Computes the logarithmic derivative of the factorial
  function defined by:
```

$$\Psi(x) = \frac{(x!)'}{x!} = \frac{\Gamma'(x+1)}{\Gamma(x+1)}.$$

```
  We make use of the expansion: (1) Ψ(x) = lnx + 1/2x −
  1/12x² + 1/120x⁴ − 1/252x⁶ + ε, (2) ε < 1/240x² and of the re-
  cursion relation, (3) Ψ(x) = Ψ(x+n) − (1/(x+1)+...+1/(x+n)).
  For x < −1 we use: (4) Ψ(−x) = πtan π(x+0.5) + Ψ(x−1).
  The value of x is increased up to a. Then Ψ is calculated by (3)
  and (1). The error is then less than 1/240a⁸;
begin real psi, pei; psi := 0;
if x > −1 ∧ x ≠ 0 then go to pos;
if x = 0 then begin psi := −0.5772156649; go to exit end;
  begin integer x1; x1 := x;
  if x = x1 then go to errexit end
  comment psi is infinite;
  pei := 3.141592654; x := −x − 1;
    psi := pei × tan(pei×(x+0.5));
pos: if x ≧ a then go to large;
  x := x + 1; psi := psi −1/x; go to pos;
large: begin real y; y := 1/x;
  psi := psi + ln(x) + y/2−y ↑ 2/12 + y ↑ 4/120−y ↑ 6/252;
exit: psif := psi;
end psif
```

CERTIFICATION OF ALGORITHM 147
PSIF [D. Amit, *Comm. ACM.*, Dec. 62]

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Reactor Eng. Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The following minor errors were noted in this algorithm:

a. (3) in the comment should read $\epsilon < 1/240\ x^8$.

b. The function *tan* is not a standard ALGOL function. It should be declared, or replaced by *sin* ( )/*cos*( ).

c. The block labelled *large* should be closed by inserting **end** immediately after 252.

The efficiency of the program would be improved by the following modifications:

a. Let the statement

if $x = 0$ **then begin** . . . **end**;

be the first statement of the procedure body.

b. Delete the condition $x \neq 0$ from the if clause,

if $x > -1 \wedge x \neq 0$ **then**. . .

c. Delete the declaration of *pei*, and the assignment of the value of 3.141592654 to *pei* in the statement

psi := *pei* × *sin*(*pei* × (*x*+0.5))/*cos*(*pei*×(*x*+0.5));

replace *pei* by the value 3.141592654.

d. Replace the block labelled large by:

large: **begin real** *y*; *x* := 1/*x*; *y* := *x* × *x*;
psi := *psi* − *ln*(*x*) + *x*/2 − ((*y*/252−0.008333333333) × *y* + 0.08333333333) × *y* **end**;

With these changes, the body of the procedure was translated and run on the LGP-30 computer using the Dartmouth SCALP processor. The program was used to tabulate *psif*(*x*) for $x = -1(0.5)0(0.005)1.250$. With $a = 3.0$ the results agreed with tabulated values to within 3 in the 6th decimal place. This is considered satisfactory, since one decimal place is lost in applying the recurrence. Running time, including output on the Flexowriter and computation of new values of the independent variable, averaged about 30 seconds per value.

It should be observed that *psif*(*x*) is $\Psi(x+1)$ as tabulated, for example, by Jahnke-Emde-Losch.

CERTIFICATION OF ALGORITHM 147 [S14]
PSIF [D. Amit, *Comm. ACM* 5 (Dec. 1962), 605]

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KEY WORDS AND PHRASES: gamma function, logarithmic derivative, factorial function, psi function
CR CATEGORIES: 5.12

The following errors were noted in this algorithm in addition to those noted by Thacher [2].

a. (4) in the comment should read "For $-x < -1$ we use: (4) $\Psi(-x) = \Psi(x-1) + \pi \cot(\pi x)$".

b. At the end of the first comment add: "Note that *psif*(*x*) ≡ $\Psi(x)$ is $\psi(x+1)$ as defined, for example, by Jahnke-Emde-Lösch" (see [1]).

c. The statement in the algorithm before the label *pos* should read: *psi* := *pei* × *cos* (*pei*×*x*)/*sin* (*pei*×*x*); These errors caused the procedure to give incorrect results for *psif*(*x*, *a*) for $x < -1$.

d. The arguments *tan* and *ln* should be deleted from the parameter list and **real procedure** *tan*, *ln*; should be deleted from the specification part of the procedure heading.

With these changes and those of Thacher, the procedure was translated into Burroughs B5500 extended ALGOL and run on the Stanford B5500. *psif*(*x*, *a*) was tabulated for $x = -2.9(0.1)5.0$ with $a = 8.0$ The results agreed with tabulated values to within $1/(240a^8)$.

REFERENCES:

1. JAHNKE-EMDE-LÖSCH. *Tables of Higher Functions* (6th Ed.). McGraw-Hill, New York, 1960.
2. THACHER, H. C., JR. Certification of Algorithm 147. *Comm. ACM 6* (Apr. 1963), 168.

ALGORITHM 148
TERM OF MAGIC SQUARE
D. M. COLLISON
Elliott Brothers (London) Ltd., Borehamwood, Herts.

```
integer procedure magicterm (x, y, n); value x, y, n; integer
  x, y, n;
comment for the magic square s[1:n, 1:n], magicterm generates
  the element s[x, y], where n > 2 and n is odd. De la Loubère's
  method is used;
begin integer b, c;
  b := y - x + (n-1) ÷ 2;  c := y + y - x;
  if b ≧ n then b := b - n else if b < 0 then b := b + n;
  if c > n then c := c - n else if c ≦ 0 then c := c + n;
  magicterm := b × n + c
end magicterm
```

CERTIFICATION OF ALGORITHM 148
TERM OF MAGIC SQUARE [D. M. Collinson, *Comm. ACM*, Dec. 1962]
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University of Alberta, Calgary; Calgary, Alberta, Canada

MAGICTERM was translated into FORTRAN for the IBM 1620. The procedure was tested for terms of squares up to order 13. Correct results were obtained. For determination of complete squares operating time was not significantly different from Algorithm 118.

CERTIFICATION OF ALGORITHM 148
TERM OF MAGIC SQUARE [D. M. Collison, *Comm. ACM*, Dec. 62]
DMITRI THORO
San Jose State College, San Jose, Calif.

This algorithm was translated into FORTRAN and FORGO for the IBM 1620. No changes in the program were necessary. The elements of magic squares of odd orders up to 15 were generated satisfactorily.

ALGORITHM 149
COMPLETE ELLIPTIC INTEGRAL

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comment The following two procedures, along with a test program were compiled and run by Peter Naur on the DISADEC computer. Compilation time for the 9 pass compiler was less than 10 seconds. The elliptic integral of the form

$$\int_0^{\pi/2} \frac{dt}{\sqrt{a^2 \cos^2 t + b^2 \sin^2 t}}$$

is evaluated by replacing a and b by their arithmetic and geometric means, respectively. *ELIP 2* is a nonrecursive procedure to accomplish the same thing;

```
real procedure ELIP 1 (a, b); value a, b; real a, b;
  ELIP 1 := if abs(a−b) <10 −8 × a
    then 3.14159265/2/a
    else ELIP 1 ((a+b)/2, sqrt (a×b));
real procedure ELIP 2 (a, b); value a, b; real a, b;
  begin real C;
  L: C := (a+b)/2; b := sqrt (a×b); a := c;
  if abs(a−b) <10 −8 × a then ELIP 2:= 3.14159265/2/a
  else go to L end
```

CERTIFICATION OF ALGORITHM 55
COMPLETE ELLIPTIC INTEGRAL OF THE FIRST KIND [John R. Herndon, *Comm. ACM*, Apr. 1961] and
CERTIFICATION OF ALGORITHM 149
COMPLETE ELLIPTIC INTEGRAL [J. N. Merner, *Comm. ACM*, Dec. 1962]

HENRY C. THACHER, JR.*
Reactor Eng. Div., Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

The bodies of Algorithm 55 and of the second procedure of Algorithm 149 were tested on the LGP-30 computer using SCALP, the Dartmouth "LOAD-AND-GO" translator for a substantial subset of ALGOL 60. The floating-point arithmetic for this translator carries 7+ significant digits.

In addition to modifications required because of the limitations of the SCALP subset, the following need correction:

In Algorithm 55:

1. The constant 0.054555509 should be 0.054544409.
2. The function *log* should be *ln*.

In procedure ELIP 2 of Algorithm 149, the statement $a := c$ should be $a := C$.

The parameters of Algorithm 149 are related to the complete elliptic integral of the first kind by: $K = a \times ELIP(a, b)$ where the parameter $m = k^2 = 1 - b/a$.

The maximum approximation error in Algorithm 55 is given by Hastings as about $0.6_{10}-6$. In addition there is the possibility of serious cancellation error in forming the complementary parameter $t = 1 - k \times k$. For k near 1, errors as great as 4 significant digits were sustained. In these regions, the complementary parameter itself is a far more satisfactory parameter.

The accuracy obtainable with Algorithm 149 is limited only by the arithmetic accuracy and the amount of effort which it is desired to expend. Six-figure accuracy was obtained with 5 applications of the arithmetic-geometric mean for $a = 1000$, $b = 2$, and with one application for $a = 500$, $b = 500$.

Neither algorithm is satisfactory for $k = 1$. The behavior for Algorithm 55 will be governed by the error exit from the logarithm procedure. Under these circumstances, Algorithm 149 goes into an endless loop. Algorithm 149 may also go into an endless loop of the terminating constant ($_{10}-8$ in the published algorithm) is too small for the arithmetic being used. For the SCALP arithmetic it was found necessary to increase this tolerance to $5.0_{10}-7$. The resulting values of the elliptic integrals were, however, accurate to within 2 in the 7th significant digit (6th decimal).

The relative efficiency of the two algorithms will depend strongly on the efficiency of the square-root and logarithm subroutines. With most systems, Algorithm 55 will provide sufficient accuracy, and will be more efficient. If a square-root operation or a highly efficient square-root subroutine is available, Algorithm 149 may well be the better method.

ACM Transactions on Mathematical Software, Vol. 4, No. 1, March 1978, Page 95.

REMARK ON ALGORITHM 149

Complete Elliptic Integral [S21]
[J.N. Merner, *Comm. ACM 5*, 12 (Dec. 1962), 605]

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The text following the colon at the end of the fifth paragraph in [4] should read as follows: $K = a \times ELIP1(a,b)$ or $K = a \times ELIP2(a,b)$, where $m = k^2 = 1 - (b/a)^2$.

A better procedure is given in [1, p. 86, *procedure cel*1]. This procedure can for some computers be made slightly more efficient by eliminating the last assignment statement $m := m/2$ in the loop, replacing the second assignment statement $m := kc + m$ with $m := (kc + m) \times .5$ and replacing the last assignment state-

ment *cel1* := *pi/m* with *cel1* := (*pi*/2)/*m*. Note the variable *m* should not be confused with the parameter $m = k^2$.

A more efficient, but less portable procedure is defined in [2] and implemented, for example, in the FUNPACK package [3].

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2. CODY, W.J. Complete elliptic integrals. In Hart, J.F., et al., *Computer Approximations*. Wiley, New York, 1968, pp. 150–154 and pp. 335–339.
3. CODY, W.J. The FUNPACK package of special function subroutines. *ACM Trans. Mathematical Software 1*, 1 (March 1975), 13–25.
4. THACHER, H.C., JR. Certification of Algorithm 149: Complete elliptic integral. *Comm. ACM 6*, 4 (April 1963), 166–167.

ALGORITHM 150
SYMINV2

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```
procedure syminv2(a,n) result: (a) exit: (fail); value n; integer n; array a; label fail;
  comment syminv2 obtains inverse of a symmetric matrix a of order n by a method which is similar to that given by Busing and Levy [Comm. ACM 5 (1962), 446] but requires no interchanges of rows and columns nor storage space for an additional matrix Q, yet is numerically equivalent. The procedure requires the upper triangular part of a to be given and overwrites it by the upper triangular part of the inverse which is again denoted by a. All pivots are chosen on the diagonal, and if all further diagonal elements which are eligible as pivots vanish (this is impossible for a positive definite matrix a) then exit through fail occurs;
  begin
    real bigajj;
    integer i, j, k;
    real array p, q[1:n];
    Boolean array r[1:n];
    for i := 1 step 1 until n do r[i] := true;
grand loop:
    for i :=1 step 1 until n do
    begin
search for pivot:
      bigajj := 0;
      for j := 1 step 1 until n do
      begin
        if r[j] ∧ abs(a[j,j]) > bigajj then
        begin
          bigajj := abs(a[j,j]);
          k := j
        end;
      end;
      if bigajj = 0 then go to fail;
preparation of elimination step i:
      r[k] := false;
      q[k] := 1/a[k,k];
      p[k] := 1;
      a[k,k] := 0;
      for j := 1 step 1 until k-1 do
      begin
        p[j] := a[j,k];
        q[j] := (if r[j] then -a[j,k] else a[j,k]) × q[k];
        a[j,k] := 0
      end;
      for j := k+1 step 1 until n do
      begin
        p[j] := if r[j] then a[k,j] else -a[k,j];
        q[j] := -a[k,j] × q[k];
        a[k,j] := 0
      end;
elimination proper:
      for j := 1 step 1 until n do
        for k := j step 1 until n do
          a[j,k] := a[j,k] + p[j] × q[k]
    end grand loop
end syminv2
```

REMARK ON ALGORITHM 150
SYMINV2 [H. Rutishauser, COMM. ACM, Feb. 1963]

ARTHUR EVANS, JR.
Carnegie Institute of Technology, Pittsburgh, Pennsylvania

The identifier "a" appears twice in the procedure heading as a formal parameter. It is not clear that this situation has any meaning in ALGOL. Indeed, it is not at all obvious how one might translate the procedure. If the actual parameters corresponding to the two formal parameters with the same identifier are different there is no way for the translator (or for the reader) to distinguish which 'a' is to be used. Further, it would take a detailed examination of the published algorithm to determine how this situation might be corrected. It is certainly not clear that it would be safe merely to delete one occurrence of the formal parameter 'a', since the operation of the algorithm might require that two separate matrices be available.

REMARK ON ALGORITHM 150
SYMINV2 [H. Rutishauser, COMM. ACM, Feb. 1963]

H. RUTISHAUSER
Eidg. Technische Hochschule, Zurich, Switzerland

procedure *syminv* 2 (*a*, *n*) result : (*a*) exit : (*fail*); ··· indicates that the value of parameter "*a*" is changed by the computing process (the matrix *a* is changed into its inverse, whereby the given matrix is destroyed). In any procedure call, the two actual parameters corresponding to the two *a*'s must be identical, otherwise the action of the procedure will be undefined (by virtue of the substitution rule). The user may also change the procedure heading into *syminv* 2 (*a*, *n*) exit : (*fail*); ··· without changing the effect of the procedure.

EDITOR'S NOTE: The ALCOR group has adopted the rule that if the value of a parameter is changed by the execution of the procedure, then the parameter should be listed twice. Although the ALGOL 60 Report does not forbid listing a formal parameter twice, it would appear that a compiler which thus restricts the language could not accept some of the examples given in the ALGOL 60 Report.

CERTIFICATION OF ALGORITHM 150
SYMINV2 [H. Rutishauser, *Comm. ACM 6* (Feb. 1963), 67]

PETER NAUR (Recd 27 Sept. 63)
Regnecentralen, Copenhagen, Denmark

Since the translator refuses to run programs with more than one occurrence of the same identifier in a formal parameter list, the second *a* was taken out when this procedure was run with the GIER ALGOL system [cf. also the discussion in *Comm. ACM 6* (July 1963), 390]. Otherwise it ran smoothly. For testing the accuracy, segments of the Hilbert matrix were inverted and the results multiplied by the original segment and compared with the unit matrix. The largest deviation in any element was found to be:

Order	*Max. deviation from elements of the unit matrix*	*Order*	*Max. deviation from elements of the unit matrix*
2	$-1.49_{10}-8$	6	$-7.32_{10}-3$
3	$-2.38_{10}-7$	7	$-3.59_{10}-1$
4	$-1.53_{10}-5$	8	-2.95_{10} 1
5	$-3.36_{10}-4$	9	-1.25_{10} 1

These figures may be compared directly with the ones related to Algorithms 120, *INVERSION II*, and *gjr* [*Comm. ACM 6* (Aug. 1963), 445]. A comparison shows that all three algorithms yield about the same accuracy, with *syminv2* being the best in most cases, however. This is not too surprising since the knowledge that the matrix is symmetric ought to simplify the calculation considerably.

The lengths of the three procedures after translation are as follows:

	Number of GIER words
syminv2	216
INVERSION II	279
gjr	302

Execution times for *syminv2* in GIER ALGOL are:

Order	*Time (sec)*
5	1
10	3.5
15	10.5
20	23

This is about half the time of execution of *INVERSION II* or *gjr*.

ALGORITHM 151
LOCATION OF A VECTOR IN A LEXICOGRAPHICALLY ORDERED LIST

HENRY F. WALTER
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```
integer procedure LOCATE (min, n, c, v, combinatorial);
value v; integer min, n, c; integer array v;
integer procedure combinatorial;
comment This procedure locates the position, LOCATE, of a
  given vector in a list of vectors without searching the list. The
  list consists of all the combinations of n consecutive digits taken
  d at a time. Min is the smallest of the n integers. Each vector
  (combination) is written in ascending order from left to right,
  as, for example, 378 and the vectors are listed lexicographically,
  by which is meant, that, considered as d digit numbers, the
  vectors are listed in ascending order. For example, with min = 1,
  d = 3, and n = 6, the vectors in order are 123, 124, 125, 126, 134,
  135, ..., 456. Given the vector, v = 356, the procedure locates
  this vector as the 19th in the list;
begin integer i, r, max, part, whole;
  r := 1;  v [0] := min - 1;  max := min - 1+n;
  for i := 0 step 1 until c-1 do
  begin part := c - i - 1;
    ask: if v[i+1] - v[i] > 1 then
      begin whole := max - v[i] - 1;
        r := r + combinatorial (whole, part);
        v[i] := v[i] + 1;
        go to ask
      end;
  end;
  locate := r
end;
```

ALGORITHM 152
NEXCOM
JOHN HOPLEY
Peat, Marwick, Mitchell & Co., London, England

```
procedure nexcom (char, N, setcomplete, nullvector);
array char; integer N;
label setcomplete, nullvector;
comment char is a column vector containing N elements each of
  which is either 1 or 0. Nexcom transforms char into another
  vector containing the same number of 1's and 0's, but in a differ-
  ent sequence. Starting with char in the state of having 1 in each of
  the element positions 1, ..., r and zeros elsewhere then repeated
  application of nexcom generates all nCr patterns of char. The
  procedure terminates if the presented vector char has 1 in each
  of the positions N, N-1, ... N-r+1 and zeros elsewhere. Termi-
  nation is indicated by exit through the formal label 'setcomplete'.
  If char is the null vector then procedure exists through the
  formal label 'nullvector';
begin integer n, p, m;
comment find the first 1 in char;
for n := 1 step 1 until N do if
char [n] = 1 then go to A;
go to nullvector;
comment how many adjacent 1's;
A: p := 0;
for m := n + 1 step 1 until N do
if char [m] = 1 then p := p + 1 else go to B;
comment Have all combinations been generated;
B: if p + n = N then go to setcomplete;
comment Set up next combination; char[n+p+1] := 1;
for m := n + p step - 1 until n do char [m] := 0;
for m := 1 step 1 until p do char [m] := 1;
end nexcom;
```

ALGORITHM 153
GOMORY

F. L. BAUER
Johannes Gutenberg-Universität, Mainz, Germany

```
procedure Gomory (a, m, n) result: (a) exit: (no solution);
  value m, n;
  integer m, n;
  integer array a;
  label no solution;
comment Gomory algorithm for all-integer programming. The
  objective of this procedure is to determine the integer solution
  of a linear programming problem with integer coefficients only.
  The tableau-matrix a consists of m + 1 rows and n columns.
  The top row of a is the objective row, the last column represents
  the right-hand sides. The tableau-columns, with the exception
  of the last column, have to be lexicographically positive. The
  algorithm is finished if all entries in the last column, except the
  top most entry, are nonnegative. Then the top most entry of
  the last column represents the value of the objective function.
  The other entries of the last column define the coordinates of
  the optimal solution. There are always the same variables con-
  nected with the same rows. The exit no solution is used if a row
  is found which has a negative entry in the last column, but
  otherwise only nonnegative entries;
begin  integer i, k, j, l, r;
       real lambda;
       integer array t[1:n-1], c[1:n];
1:     for i := 1 step 1 until m do if a[i,n] < 0 then
       begin r := i;  go to 2 end;
       go to end;
2:     for k := 1 step 1 until n-1 do if a[r,k] < 0 then
       go to 4;
       go to no solution;
4:     l := k;
       for j := k+1 step 1 until n-1 do if a[r,j] < 0 then
         begin i := 0;
           3:  if a[i,j] < a[i,l] then l := j else
               if a[i,j] = a[i,l] then
               begin i := i+1;  go to 3 end
         end;
       for j := 1 step 1 until n-1 do if a[r,j] < 0 then
         begin if a[0,l] ≠ 0 then t[j] := entier(a[0,j]/a[0,l])
           else t[j] := 1
         end;
       lambda := abs(a[r,1]/t[1]);
       for j := 2 step 1 until n-1 do if a[r,j] < 0 then
         begin if abs(a[r,j]/t[j]) > lambda then
           lambda := abs(a[r,j]/t[j]) end;
       for j := 1 step 1 until n do if j≠l then
         begin c[j] := entier(a[r,j]/lambda);
           if c[j] ≠ 0 then
           for i := 0 step 1 until m do a[i,j] := a[i,j] + c[j] ×
             a[i,l]
         end;
       go to 1;
end:   end;
```

CERTIFICATION OF ALGORITHM 153
GOMORY [F. L. Bauer, *Comm. ACM 6*, Feb. 1963]

B. LEFKOWITZ AND D. A. D'ESOPO*
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* Work supported by Office of Naval Research.

GOMORY was hand-coded in BALGOL for the Burroughs 220 and in FORTRAN for the CDC 1604. The following corrections should be made:

The statement

```
  lambda := abs(a[r,1]/t[1]);
```

should read

```
  lambda := abs(a[r,l]/t[l]);
```

The statement

```
  for j := 2 step 1 until n-1 do if a[r,j] < 0 then
```

should read

```
  for j := 1 step 1 until n-1 do if a[r,j] < 0 then
```

The following changes to Bauer's program were made to increase its efficiency and reduce storage requirements.

Change the statement

```
  begin integer i, k, j, 1, r;
```

to read

```
  begin integer i, k, j, 1, r, c, t;
```

Change the statement

```
  real lambda;
```

to read

```
  real lambda, lambd;
```

Delete the statement

```
  integer array t[1: n-1], c[1: n];
```

Before the statement

```
  for j := 1 step 1 until n-1 do if a[r,j] < 0 then
```

insert the statement

```
  lambda := 1.0;
```

Change the statement

```
  begin if a[0,l] ≠ 0 then t[j] := entier(a[0,j]/a[0,l])
```

to read

```
  begin if a[0,l] ≠ 0 then t := entier(a[0,j]/a[0,l])
```

Change the statement

```
  else t[j] := 1
```

to read

```
  else t := 1
```

After the statement

```
  else t[j] := 1
```

insert the statements

```
  lambd := -a[r,j]/t;
  lambda := if lambda < lambd then lambd else lambda;
```

Delete the statements starting with

```
  lambda := abs(a[r,1]/t[1]);
```

up to and including

```
  lambda := abs(a[r,j]/t[j]) end;
```

Change the statement

```
  begin c[j] := entier (a[r, j]/lambda);
```

to read

```
  begin c := entier(a[r,j]/lambda);
```

Change the statement

```
  if c[j] ≠ 0 then
```

to read

```
  if c ≠ 0 then
```

Change the statement

```
  for i := 0 step 1 until m do a[i,j] := a[i,j] + c[j] ×
```

to read

for $i := 0$ **step** 1 **until** m **do** $a[i,j] := a[i,j] + c \times$

The "tie-breaking" procedure embodied in the three statements beginning at

$$3: \textbf{if } a[i,j] < a[i,l] \textbf{ then } l := j \textbf{ else}$$

will fail if the two columns being compared are identical. Although this cannot happen on the first iteration, it may occur later. To test for this condition change the two statements beginning with

$$\textbf{begin } i := i + 1; \quad \textbf{go to } 3 \textbf{ end}$$

to read

begin $i := i + 1$; **if** $i > m$ **then go to** 31 **else go to** 3 **end**;
31: **end**;

The revised algorithm yielded satisfactory answers on a ten equation-seven variable problem in 159 iterations and a 35-equation 14-variable problem in 447 iterations.

The following comments may be helpful for preparing a problem for GOMORY. The problem constraints must be stated in the form:

$$\sum_j a_{ij}x_j + s_i = b_i$$

where the s_i are slack variables. The columns representing these slack variables need not appear in the initial tableau-matrix a.

Since the only variables in the solution that will necessarily be non-negative are the s_i, any non-negativity constraints on the other variables must be among the above equations (e.g. the constraint $x_j \geqq 0$ is represented by $-x_j + s_k = 0$).

The size of the integers in the b vector substantially affects the number of iterations.

The requirement that all but the last tableau-columns be lexicographically positive means that the first nonzero element in these columns must be positive.

EDITOR'S NOTE: Prof. Bauer wishes to indicate that for the Algorithm 153, GOMORY, credit is due to Ch. Witzgall, who wrote the draft.

ALGORITHM 154
COMBINATION IN LEXICOGRAPHICAL ORDER

CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

```
procedure COMB1 (n,r,I); integer n, r; integer array I;
comment The distinct combinations of the first n integers
  taken r at a time are generated in I in lexicographical order
  starting with an initial combination of the r integers 1, 2, ··· ,
  r. Each call of the procedure, after the first, must have in I
  the previous generated combination. The Boolean variable
  first is nonlocal to COMB1 and must be true before the first call.
  Thereafter first remains false until all combinations have been
  generated. When calling COMB1 with I containing n − r + 1,
  n − r + 2, ··· , n, I is left unchanged and first is set true;
begin integer s, j;
  if first then begin for j := 1 step 1 until r do
    I[j] := j;
    first := false; go to EXIT end;
  begin if I[r] < n then begin I[r] := I[r] + 1; go to EXIT
          end;
    for j := r step −1 until 2 do
      if I[j−1] < n − r + j − 1 then
        begin I[j−1] := I[j−1] + 1;
          for s := j step 1 until r do
            I[s] := I[j−1] + s − (j−1); go to EXIT end end;
  first := true;
EXIT : end
```

CERTIFICATION OF ALGORITHM 154
COMBINATION IN LEXICOGRAPHICAL ORDER

[Charles J. Mifsund, *Comm. ACM*, Mar. 1963]

K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

This procedure was tested

for r := 1 **step** 1 **until** n with n = 6

with correct results.

ALGORITHM 155
COMBINATION IN ANY ORDER
CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

```
procedure COMB2 (m,M,n,r,s,S,TOTAL); integer array m,
          M, S; integer n, r, s,TOTAL;
comment Each call of COMB2 generates a distinct combination
  S, (if possible) of the n integer values of J taken r (r>1)
  at a time if J consists of m[1] integers each equal to M[1], and
  m[2] integers each equal to M[2], and so on, there being s integers
  available. TOTAL must be set to zero before the first call of
  COMB2 and thereafter TOTAL is increased by one after each
  new combination is generated. To speed up the machine operation arrange the s integers in M such that m[1] ≧ m[2] ≧ ··· ≧
  m[s];
begin integer i, j, t, p; own integer array J[1:n], I[1:r]; own
Boolean first;
  if TOTAL = 0 then begin
    t := 1; p := 0;
    for j := 1 step 1 until s do
      begin p := p + m[j];
        for i := t step 1 until p do
          begin J[i] := M[j];
            t := t + 1 end end;
              first := true end;
  1: COMB1 (n,r,I);
     if first then go to EXIT;
       if I[1] = 1 then go to 2 else go to 3;
  2: for j := 2 step 1 until r do
     if (J[I[j]]=J[I[j]-1]) ∧ (I[j]>I[j-1]+1) then go to 1;
       go to 4;
  3: if J[I[1]] = J[I[1]-1] then go to 1 else go to 2;
  4: for j := 1 step 1 until r do
       S[j] := J[I[j]];
     TOTAL := TOTAL + 1;
EXIT: end
```

CERTIFICATION OF ALGORITHM 155
COMBINATION IN ANY ORDER [Charles J. Mifsud, *Comm. ACM*, Mar. 1963]
K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

This procedure was tested using

$$m[1] = 4 \quad m[2] = 3 \quad m[3] = 2 \quad m[4] = 2$$

$$M[1] = 4 \quad M[2] = 7 \quad M[3] = 9 \quad M[4] = 16$$

and **for** $r := 1$ **step** 1 **until** s

It is correctly generated for $r = 1$ the four combinations 4, 7, 9, 16, as well as the ten combinations for $r = 2$, the eighteen combinations for $r = 3$, and the twenty-six combinations for $r = 4$.

Changes made due to compiler limitations were (i) systematic changes of upper case letters where there was conflict due to having only one case of letters, (ii) transfer of **own** declared variables to non-local variables, and (iii) integer labels to identifiers.

ALGORITHM 156
ALGEBRA OF SETS
CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

```
procedure INOUT (A,n,SUM); real array A; integer n;
          real SUM;
comment SUM = Σ1 Ai − Σ2 AiAj + Σ3 AiAjAk − ··· ±
  A1A2 ··· An is formed where the symbols Σ1, Σ2, Σ3, ···,
  Σn−1 stand for summation of the possible combinations of the
  numbers A1, A2, ···, An taken one, two, three, ···, (n−1)
  at a time;
  begin real j, part, T; integer i, r; integer array I[1:n];
  Boolean first;
    r := SUM := 0; j := − 1;
  B: first := true; r := r + 1; part := 0;
  A: COMB1 (n,r,I);
      if first then begin j := −1 × j; part := j × part;
        SUM := SUM + part;
        if r < n then go to B else go to EXIT end;
      T := 1;
      for i := 1 step 1 until r do
        T := A[I[i]] × T;
      part := part + T; go to A;
EXIT: end
```

CERTIFICATION OF ALGORITHM 156
ALGEBRA OF SETS [Charles J. Mifsud, *Comm. ACM*, Mar. 1963]
K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

One correction required in this procedure is the systematic change of label *A* to avoid conflict with the formal parameter array *A*.

The procedure was then tested for $n = 9$ and $Ai = i$, $i = 1, \cdots, n$, producing the correct answer $SUM = 1$.

Two other tests with arbitrary values of Ai and $n = 4$ were also correct.

ALGORITHM 157
FOURIER SERIES APPROXIMATION

CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

```
procedure FOURIER (N,f,a,b); real array f, a, b; integer N;
comment Fourier determines 2N+1 constants a_p (p=0,1,···,N),
  b_p (p=1,2,···,N) in such a way that the equations f_n = 1/2a_0 +
  Σ_{p=1}^{N}(a_p cos 2πnp/(2N+1) + b_p sin 2πnp/(2N+1)) are satisfied,
  where the f_n are given numbers. The f_n may be thought of as the
  2N+1 values of a function f(x) at the points x_n = 2πn/(2N+1).
  The method used to generate a_p , b_p was formulated by G.
  Goertzel in "Mathematical Methods for Digital Computers"
  (John Wiley and Sons, Inc., 1960);
begin real array S, C[1:2], u[0:2]; real TEMP, pi;
  integer p, i;
  pi := 3.14159265; C[2] := 1; S[2] := 0;
  C[1] := cos(2×pi/(2×N+1));
  S[1] := sin(2×pi/(2×N+1));
  for p := 0 step 1 until N do
    begin u[1] := u[2] := 0;
      for i := 2 × N step −1 until 1 do
        begin u[0] := f[i] + 2 × C[2] × u[1] − u[2];
          u[2] := u[1]; u[1] := u[0]end;
    a[p] := 2/(2×N+1) × (f[0]+u[1]×C[2]−u[2]);
    b[p] := 2/(2×N+1) × u[1] × S[2];
    TEMP := C[1] × C[2] − S[1] × S[2];
    S[2] := C[1] × S[2] + S[1] × C[2];
    C[2] := TEMP end end
```

REMARK ON ALGORITHM 157
FOURIER SERIES APPROXIMATION [C. J. Mifsud, *Comm ACM*, Mar. 1963]

RICHARD GEORGE*
Argonne National Laboratory, Argonne, Ill.

This algorithm was written in FAP language for the 32-K IBM 704. It was tested on a sawtooth curve, and the sawtooth was recreated by summing the expansion up through the $2N + 1$ constants, with excellent results.

* Work supported by the United States Atomic Energy Commission.

The arrays S, C and u are never referenced with a variable subscript. For a saving of time, I suggest that simple variables be used instead.

By declaring one additional real variable, one can bring the phrase

$$2/(2 \times N + 1)$$

outside of the **for** loops, because N does not change through the procedure. This results in a saving of $4N+2$ mult-ops.

REMARK ON ALGORITHM 157
FOURIER SERIES APPROXIMATION [Charles J. Mifsud, *Comm. ACM*, Mar. 1963]

GEORGE R. SCHUBERT*
University of Dayton, Dayton, Ohio

* Undergraduate research project, Computer Science Program, Univ. of Dayton.

Algorithm 157 has been modified to fit $2N$ data points and has run successfully on the Burroughs 220 using BALGOL. With the modifications, $2N$ constants a_p ($p=0, 1, \cdots, N$) and b_p ($p=1, 2, \cdots, N-1$) are determined such that the equation $f_n = a_0/2 + \sum_{p=1}^{N-1} (a_p \cos \pi np/N + b_p \sin \pi np/N) + a_N/2 \cos \pi n$ is satisfied.

In the modified procedure, the second and third lines after the integer declaration should read:

```
C[1] := cos (pi/N);
S[1] := sin (pi/N);
```

The second **for** statement should read:

```
for i := 2 × N−1 step −1 until 1 do
```

The lines containing the a and b coefficients should read:

```
a[p] := (f[0]+u[1]×C[2]−u[2])/N;
b[p] := (u[1]×S[2])/N;
```

REFERENCE: R. W. Hamming, *Numerical Methods for Scientists and Engineers*, pp. 68–73 (McGraw-Hill, 1962).

ALGORITHM 158 (ALGORITHM 134, REVISED) EXPONENTIATION OF SERIES

HENRY E. FETTIS
Aeronautical Research Laboratories, Wright-Patterson Air Force Base, Ohio

```
procedure SERIESPWR (A,B,P,N); value A, P, N;
          array A, B; integer N;
comment This procedure calculates the first N coefficients
  B[i] of the series g(x) = f(x) ↑ P given the first N coefficients
  of the series

      f(x) = 1 + Σ A[i] × x ↑ i      (i=1,2,-,-,N).

  P may be any real number. Setting P := 0 gives the coefficients
    for LN(g(x));
  begin integer i, k;
  real P, S;
    if P = 0 then B[1] = A[1];
else B[1] := P × A[1];
  for i := 2 step 1 until N do
  begin S := 0;
    for k := 1 step 1 until i - 1 do
    S := S + (P×(N-k)-k) × B[k] × A[N-k];
    B[i] := P × A[i] + (S/i)
      end for i;
end SERIESPWR
```

CERTIFICATION OF ALGORITHM 158 EXPONENTIATION OF SERIES [H. E. Fettis, *Comm. ACM*, Mar. 1963]

J. DENNIS LAWRENCE
Lawrence Radiation Laboratory, Livermore, Calif.

This procedure was translated into FORTRAN and run on the Remington-Rand LARC Computer. Three changes are necessary.

(1) The last line of the comment should read

for the natural logarithm of $f(x)$;

(2) The third line from the end should read

$$S := S+(P\times(i-k)-k)\times B[k]\times A[i-k];$$

(This line was given correctly in algorithm 134.)

(3) The second line from the end apparently should read

$$B[i] := A[i] := (S/i);$$

for the case $P = 0$ only. Probably the best way to incorporate this is by making two changes:

(a) Change the **if** clause to read

if $P = 0$ **then** $R := 1$ **else** $R := P$; $B[1] := R \times A[1]$;

(b) Change the second line from the end to read

$$B[i] := R \times A[i] + (S/i);$$

A large number of examples were run quite successfully; the following give representative samples.

(1) $(1+2x+3x^2+0.5x^3)^2 = 1+4x+10x^2+13x^3+11x^4+3x^5+0.25x^6$ (using $A[4] := A[5] := A[6] := 0$).

(2) Setting $P := 1$ gives $B[i] := A[i]$.

(3) Let $f(x) = e^x = 1 + \sum_{i=1}^{n} \frac{1}{i!} x^i$ and let $P = ln2 = .693147181$. Then $g(x) = 2^x = 1 + \sum_{i=1}^{n} \frac{(ln2)^i}{i!} x^i$. (See Table 1.)

(4) Let $f(x)=e^x$ and $P=-1$. Then $g(x)=e^{-x}$. For $P=0$, apparently the constant term of $g(x)$ should be zero instead of one.

TABLE 1

	A[i]	B[i]
1	1.000000000	0.693147181
2	0.500000000	0.240226507
3	0.166666667	0.055504109
4	0.041666667	0.009618129
5	0.008333333	0.001333356
6	0.001388889	0.000154035
7	0.000198413	0.000015253
8	0.000024802	0.000001322
9	0.000002756	0.000000102
10	0.000000276	0.000000007

(5) Let $f(x)=e^x$ and $P=0$. Then $g(x)=x$.

(6) Let $f(x)=\sum_{i=0}^{n} x^n$ and $P=0$. Then $g(x)=ln(1-x^n)-ln(1-x)=\sum_{i=1}^{n} \frac{1}{i} x^i$. (See Table 2.)

TABLE 2

	A[i]	B[i]
1	1.0	1.000000000
2	1.0	0.500000000
3	1.0	0.333333340
4	1.0	0.250000000
5	1.0	0.200000000
6	1.0	0.166666670
7	1.0	0.142857140
8	1.0	0.125000000
9	1.0	0.111111110
10	1.0	0.100000000
11	1.0	0.090909100
12	1.0	0.083333330
13	1.0	0.076923080
14	1.0	0.071428580
15	1.0	0.066666660

CERTIFICATION OF ALGORITHMS 134 AND 158 EXPONENTIATION OF SERIES [Henry E. Fettis, COMM. ACM, Oct. 1962 and Mar. 1963]

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Reactor Engineering Div., Argonne National Laboratory
Argonne, Ill.

Work supported by the U.S. Atomic Energy Commission.

The bodies of SERIESPWR were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. In addition to the modifications required by the limitations of this translator, the following corrections were necessary:

1. Add "**real** P;" to the specifications.
2. Delete "p," from the declarations in the procedure body.
3. (134 only) Replace "S" by "s" and $[i-k]$ by "$(i-k)$" in the statement $S := s + \cdots$.
4. (158 only) Changes last sentence of comment to "Setting $P := 0$ gives the coefficients for $ln(f(x))$. In this series, the constant term is 0, instead of 1 as elsewhere;"
5. (158 only) Add the identifier $P2$ to the declared real variables.
6. (158 only) Make the first statements read:
   "**if** $P = 0$ **then** $P2 := 1$ **else** $P2 := P$;
   $B[1] := P2 \times A[1]$;
7. (158 only) Make the statement of the **for** k loop read

   "$S := S+(P\times(i-k)-k) \times B[k] \times A[i-k]$;"

8. Change the last statement to

   "$B[i] := P2 \times A[i] + S/i$ **end** for i;

In addition, the following modifications would improve the efficiency of the program:

1. Remove A from the value list.
2. Omit the statement $B[1] := P \times A[1]$; ($P2\times A[1]$ in 158 according to correction 6) and change the initial value of i in the statement following from 2 to 1.

When these changes were made, both procedures produced the first ten coefficients of the series for $(exp(x)) \uparrow 2.5$ from the first ten coefficients of the exponential series. The procedures were also used to generate the binomial coefficients by applying them to $(1+x)^P$, for $P = 2.0$, and 0.5000000. Algorithm 158 was also tested with $P := 0$ for $1+x$ and for the series expansions for $(sin\ x)/x$, $cos\ x$, and $exp\ x$. In all cases, the coefficients agreed with known values within roundoff.

ALGORITHM 159
DETERMINANT

DAVID W. DIGBY
Oregon State University, Corvallis, Ore.

```
real procedure Determinant (X,n);
value n; integer n; array X;
comment Determinant calculates the determinant of the n-by-
  n square matrix X, using the combinatorial definition of the
  determinant. This algorithm is intended as an example of a
  recursive procedure which is somewhat less trivial than Factorial
  (Algorithm 33);
begin real D; integer i; Boolean array B[1:n];
  procedure Thread (P,e,i);
    value P, e, i; real P; integer e, i;
    if i > n then D := D + P × (−1) ↑ e else if P ≠ 0 then
      begin integer j, f;
        f := 0;
        for j := n step −1 until 1 do
          if B[j] then f := f + 1 else
            begin
              B[j] := true;
              Thread (P×X[i,j],e+f,i+1);
              B[j] := false;
            end of loop;
      end of Thread;
  for i := 1 step 1 until n do
    B[i] := false;
  D := 0;
  Thread (1,0,1);
  Determinant := D;
end Determinant;
```

CERTIFICATION OF ALGORITHM 159
DETERMINANT [David W. Digby, *Comm. ACM*, March 1963]

ARNOLD LAPIDUS
Courant Institute of Mathematical Sciences, New York University, New York, N. Y.

Algorithm 159 was translated into FORTRAN II for the IBM 7090 as part of a test of FORTRAN subroutines designed to facilitate the implementation of recursive procedures. As expected, the numerical results were poor. For the Hilbert matrices $H_n = (a_{ij})$, $a_{ij} = 1/(i+j-1)$, results were as follows:

n	Det H_n (true)	Det H_n (computed by Algorithm 159)
2	8.333 333 3 (− 2)	8.333 333 2 (− 2)
3	4.629 629 6 (− 4)	4.629 623 1 (− 4)
4	1.653 439 2 (− 7)	1.651 933 4 (− 7)
5	3.749 295 1 (−12)	−2.910 383 0 (−11)

Determinants of order 4 and 6 with integer elements were also evaluated. The algorithm gave full accuracy for these.

ALGORITHM 160
COMBINATORIAL OF M THINGS TAKEN N AT A TIME

M. L. WOLFSON AND H. V. WRIGHT
United States Steel Corp., Monroeville, Penn.

```
integer procedure combination (m, n);
value n; integer m, n;
comment calculates the number of combinations of m things
  taken n at a time. If n is less than half of m, then the program
  calculates the combinations of m things taken m − n at a time
  which is the exact equivalent of m things taken n at a time;
begin integer p, r, i;
  p := m − n;
  if n < p then begin p := n; n := m − p end;
  if p = 0 then begin r := 1; go to exit end;
  r := n + 1;
  for i := 2 step 1 until p do r := (r × (n+i))/i;
exit: combination := r
end combination
```

CERTIFICATION OF ALGORITHM 160
COMBINATORIAL OF *M* THINGS TAKEN *N* AT A TIME [M. L. Wolfson and H. V. Wright, *Comm. ACM*, Apr. 1963]

DMITRI THORO
San Jose State College, San Jose, Calif.

Algorithm 160 was translated into FORTRAN II and FORGO for the IBM 1620. Correct results were obtained for values of m up to 20.

CERTIFICATION OF ALGORITHM 160
COMBINATORIAL OF M THINGS TAKEN N AT A TIME [M. L. Wolfson and H. V. Wright, *Comm. ACM*, April 1963]

ROBERT F. BLAKELY
Indiana Geological Survey, Bloomington, Ind.

Algorithm 160 was translated into ALGO, a compiler for the Control Data Corp. G-15 computer (formerly the Bendix G-15).

With the restriction that $m \geqq n \geqq 0$, correct results were obtained for all integer values of m and n, where $0 \leqq m \leqq 10$. Several other values were tested and all results were correct.

ALGORITHM 161
COMBINATORIAL OF M THINGS TAKEN ONE AT A TIME, TWO AT A TIME, UP TO N AT A TIME

H. V. WRIGHT AND M. L. WOLFSON
United States Steel Corp., Monroeville, Penn.

```
procedure combination vector (m, n, v);
integer m, n; integer array v;
comment calculates all combinations of m things taken from 1
  to n at a time. The result is a vector, v, within which the first
  element is the combination of m things taken 1 at a time, the
  second element is the combinations of m things taken 2 at a time,
  the third element taken 3 at a time, ···, and the nth element
  taken n at a time.
begin integer i;
  v[1] := m;
  for i := 2 step 1 until n do
    v[i] := (v[i-1] × (m-i+1))/i;
end combination vector
```

CERTIFICATION OF ALGORITHM 161
COMBINATORIAL OF *M* THINGS TAKEN ONE AT A TIME, TWO AT A TIME, UP TO *N* AT A TIME

[H. V. Wright and M. L. Wolfson, *Comm. ACM*, Apr. 1963]

DMITRI THORO
San Jose State College, San Jose, Calif.

Algorithm 161 was translated into FORTRAN II and FORGO for the IBM 1620. Correct results were obtained for values of m up to 20.

CERTIFICATION OF ALGORITHM 161
COMBINATORIAL OF M THINGS TAKEN ONE AT A TIME, TWO AT A TIME, UP TO N AT A TIME

[H. V. Wright and M. L. Wolfson, *Comm. ACM*, Apr. 1963]

DAVID H. COLLINS
Indiana Geological Survey, Bloomington, Ind.

Algorithm 161 was translated into ALGO, a compiler for the Control Data Corp. G-15 computer (formerly the Bendix G-15).

With the restriction that $m \geqq n \geqq 1$, correct results were obtained for all integer values of m and n, where $1 \leqq m = n \leqq 15$. Several other values were tested (including cases where $m \neq n$) and all results were correct.

ALGORITHM 162
XYMOVE PLOTTING

FRED G. STOCKTON
Shell Development Co., Emeryville, Calif.

```
procedure xymove (XZ, YZ, XN, YN); value XZ, YZ, XN, YN;
integer XZ, YZ, XN, YN;
comment xymove computes the code string required to move the
  pen of a digital incremental X,Y-plotter from an initial point
  (XZ, YZ) to a terminal point (XN, YN) by the "best" approxi-
  mation to the straight line between the points. The permitted
  elemental pen movement is to an adjacent point in a plane
  Cartesian point lattice, diagonal moves permitted. The eight
  permitted pen movements are coded

      1 = +Y,  2 = +X+Y,  3 = +X,  4 = +X-Y,
      5 = -Y,  6 = -X-Y,  7 = -X,  8 = -X+Y.

  The approximation is "best" in the sense that each point tra-
  versed is at least as near the true line as the other candidate
  point for the same move.
  xymove does not use multiplication or division.;
begin integer A, B, D, E, F, T, I, move;
comment code (J) is a procedure which returns a value of code
  according to the following table:

      J     1  2  3  4  5  6  7  8
      code  1  2  3  2  3  4  5  4
      J     9 10 11 12 13 14 15 16
      code  5  6  7  6  7  8  1  8

  plot (move) is a procedure which sends move to the plotter as a
  plotter command.;
    if XZ = XN ∧ YZ = YN then go to return;
    A := XN - XZ; B := YN - YZ; D := A + B; T :=
    B - A; I := 0;
    if B ≧ 0 then I := 2;
    if D ≧ then I := I + 2;
    if T ≧ 0 then I := I + 2;
    if A ≧ 0 then I := 8 - I else I := I + 10;
    A := abs(A); B := abs(B); F := A + B; D := B - A;
    if D ≧ 0 then begin T := A; D := -D end else T := B;
    E := 0;
  repeat: A := D + E; B := T + E + A;
          if B ≧ 0 then begin E := A; move := code(I);
          F := F - 2 end
          else begin E := E + T; F := F - 1;
          move := code(I-1) end;
          plot(move);
          if F > 0 then go to repeat;
  return:
end
```

CERTIFICATION OF ALGORITHM 162
XYMOVE PLOTTING [Fred G. Stockton, *Comm. ACM*, Apr. 1963]

WILLIAM E. FLETCHER
Bolt, Beranek and Newman Inc., Los Angeles, Calif.

The line in the body of the procedure which read:

```
if D ≧ then I := I + 2;
```

was corrected to read:

```
if D ≧ 0 then I := I + 2;
```

With this one change the body of the procedure was transliterated into DECAL-BBN and successfully run on a PDP-1 computer utilizing the cathode ray tube output to display the path of a simulated digital incremental plotter.

REMARK ON ALGORITHM 162 [J6]
XYMOVE PLOTTING [F. G. Stockton, *Comm. ACM 6* (Apr. 1963), 161; *6* (Aug. 1963), 450]

D. K. CAVIN (Recd. 10 Feb. 1964)
Oak Ridge National Laboratory, Oak Ridge, Tenn.

The following modifications were made to Algorithm 162 to decrease the average execution time. The last nine lines of Algorithm 162 are replaced by the following:

```
          move := code(I-1); I := code(I);
  repeat: A := D + E; B := T + E + A;
          if B ≧ 0 then begin E := A; F := F - 2; plot(I) end
            else begin E := E + T; F := F - 1; plot(move) end;
          if F > 0 then go to repeat;
  return:
end
```

It is obvious that on any movement containing more than two elemental pen movements the use of the code procedure in the loop is redundant, since no more than two of the eight permitted pen movements are necessary for the approximation of any line. Therefore moving the call of the code procedure outside of the basic loop reduces the execution time whenever the X, Y movement requires more than two elemental pen movements. The procedures were coded in CODAP, the assembly language for the CDC 1604-A, and this modified version was approximately 40 percent faster in the loop than the original version. The timing comparisons used numbers in the range −2000 to 2000 with heavy emphasis on the subrange −150 to 150. The typographical error noted in the certification (*Comm. ACM*, August 1963) was corrected in both codes.

[A referee verifies that Algorithm 162 does indeed run, as changed.—G.E.F.]

ALGORITHM 163
MODIFIED HANKEL FUNCTION

HENRY E. FETTIS
Aeronautical Research Laboratories, Wright-Patterson Air Force Base, Ohio

```
procedure EXPK (P, X, E); real P, X, E;
comment this procedure calculates the modified Hankel Function e^x K_p(x) to within a given accuracy E from the integral representation:
        e^x K_p(x) = ∫_0^∞ e^{x(1-cosh t)} cosh(pt) dt;
begin real F, G, H, R, S, T, U, Y, Z, ZP;
  R := 0.0;
H := 1.0;
    iteration: begin
        G := R;
        T := .5 × H;
        S := 0;
        Z := exp(T);
        U := Z × Z;
          integration: begin
            Y := X × (1−.5×(Z+1/Z));
            if P = 0 then ZP := 1
            else ZP := Z ↑ P;
            F := .5 × exp(Y) × (ZP+1/ZP);
            S := S + F;
            Z := Z × U;
            end;
            if F ≧ E then go to integration
            else R := H × S;
            H := .5 × H;
          end;
        if abs (R−G) ≧ E then go to iteration
        else EXPK: = R
  end EXPK
```

The algorithm was found to be excessively slow. Times on the LGP-30 were of the order of 6 minutes. A considerable saving in time could be realized by improving the quadrature formula, currently the simple midpoint formula, repeated completely for each iteration. A more effective method would be a modified Romberg algorithm. A procedure based on the latter approach is being developed in this division.

* Work supported by the U. S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 163
MODIFIED HANKEL FUNCTION [Henry E. Fettis, *Comm. ACM*, Apr. 1963]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

Since this algorithm is a function declaration, the procedure declaration should be:

```
real procedure EXPK(D, X, E); ···
```

Otherwise, no syntactical errors were noticed.

The body of the procedure was translated and run on the LGP-30 computer, using the Dartmouth SCALP system. Results for $E = 0.0001$, $X = 0.1(0.1)1.0$, $P = 0$, 0.3333333, 0.6666667 and 1.000000 agreed with values tabulated in Jahnke-Emde-Losch to the 3-4D given in the tables, except for errors discovered in the table of $2/\pi K_{2/3}(x)$.

With $X = 0$, the program ended in floating-point overflow. The algorithm itself, or the call of the procedure, should include a test to insure that the variable is greater than *eps*, where *eps* is chosen to prevent exceeding machine capacity.

ALGORITHM 164
ORTHOGONAL POLYNOMIAL LEAST SQUARES SURFACE FIT

R. E. CLARK, R. N. KUBIK, L. P. PHILLIPS
The Babcock & Wilcox Co., Atomic Energy Div., Lynchburg, Va.

procedure *surfacefit* (*x, u, y, w, z, nmax, mmax, imax, jmax*)
result: (*beta, phi, zcomp, minsqd, minsqdcomp, sumdifcomp, maxdifcomp*);
real array *x, u, y, w, z, phi, beta, zcomp*;
integer *nmax, mmax, imax, jmax*;
real *minsqd, minsqdcomp, sumdifcomp, maxdifcomp*;
comment this is a transliteration of an operating program written in Burroughs ALGOL for the B-220. It fits, in the least squares sense, a polynomial function of two independent variables to values of a dependent variable specified at points on a rectangular grid in the plane of the independent variables. The use of orthogonal polynomials leads to a particularly simple system of linear equations rather than the ill-conditioned system which arises from the usual normal equations. It also provides a measure of the improvements resulting from each new term included which further leads, in this algorithm, to an automatic selection of a "best" degree polynomial function as determined by Gauss' criterion. The initial normalization of the variables results in significant reduction of round off errors in many cases. This algorithm is developed more fully in BAW-182. For a very similar approach to this and related problems see Cadwell, J. H., "Least Squares Surface Fitting Program", *The Computer J. 3* (1961), 266 and Cadwell, J. H., and Williams, D. E., "Some Orthogonal Methods of Curve and Surface Fitting," *The Computer J. 4* (1961), 260. A further reference is Gauss, C. F., "Theoria Combinationis Observationum Erroribus Minimis Obnoxial," *Gauss Werke 4* (Gottingen 1873), 3-93. *x[i]* and *y[j]* are the independent variables, *z[i, j]* is the dependent variable. *u[i]* and *w[j]* represent the weights corresponding to *x[i]* and *y[j]*, respectively. *nmax* is one more than the maximum degree of *x* to be considered. *mmax* is one more than the maximum degree of *y* to be considered. *imax* is the number of *x*'s, and *jmax* is the number of *y*'s. *beta[n, m]* is a measure of the improvement resulting from the inclusion of the $x^n y^m$th term. *phi[n, m]* is the polynomial coefficient for the $x^n y^m$th term. Note the degree of the resulting polynomial may be less than the maximum degree specified as a result of the application of Gauss' criterion. *zcomp* is the computed dependent variable.

$$minsqd = \left(\frac{\sum_{i,j} u[i] \cdot w[j] \cdot z[i,j]^2 - \sum_{n,m} beta[n,m]}{imax \cdot jmax} \right)^{1/2}$$

$$minsqdcomp = \left(\frac{\sum_{i,j} u[i] \cdot w[j] (z[i,j] - zcomp[i,j])^2}{imax \cdot jmax} \right)^{1/2}$$

$$sumdifcomp = \frac{\sum_{i,j} | z[i,j] - zcomp[i,j] |}{imax \cdot jmax}$$

$$maxdifcomp = max \, | z(i,j) - zcomp((i,j) |$$

minsqd and *minsqdcomp* are equal if computation is exact. In practice they will not be equal due to the imprecise nature of calculation. A wide discrepancy indicates excessive errors in calculation;

```
begin
real array a, b, denpa[1:nmax], c, d, denqa[1:mmax],
  alpha[1:nmax, 1:mmax], p[1:nmax, 1:imax], q[1:mmax, 1:jmax],
  pc[1:nmax, 1:nmax], qc[1:mmax, 1:mmax];
integer n, m, i, j, s, t, r;
real sumx, sumy, sumz, meanx, meany, meanz, numa, dena, denb,
  numc, denc, dend, alph, sumzsq, gausscrit, trialgausscrit, betasum,
  rescomp, poly;
comment normalization of variables;
sumx := sumy := sumz := 0.0;
for i := 1 step 1 until imax do
  sumx := sumx + x[i];
meanx := sumx/imax;
for i := 1 step 1 until imax do
  x[i] := x[i] - meanx;
for j := 1 step 1 until jmax do
  sumy := sumy + y[j];
meany := sumy/jmax;
for j := 1 step 1 until jmax do
  y[j] := y[j] - meany;
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do
    sumz := sumz + z[i,j] end;
meanz := sumz/(imax × jmax);
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do
    z[i, j] := z[i, j] - meanz end;
comment evaluate orthogonal polynomials;
numa := dena := 0.0;
for i := 1 step 1 until imax do begin
  p[1, i] := 1.0;
  numa := numa + u[i] × x[i];
  dena := dena + u[i] end;
a[2] := numa/dena;
for i := 1 step 1 until imax do
  p[2, i] := x[i] - a[2];
for n := 3 step 1 until nmax do begin
  numa := dena := denb := 0.0;
  for i := 1 step 1 until imax do begin
    numa := numa + u[i] × x[i] × p[n-1] ↑ 2;
    dena := dena + u[i] × p[n-1, i] ↑ 2;
    denb := denb + u[i] × p[n-2, i] ↑ 2 end;
    a[n] := numa/dena; b[n] := dena/denb;
    for i := 1 step 1 until imax do
      p[n, i] := (x[i]-a[n]) × p[n-1, i] - b[n] × p[n-2, i] end;
  numc := denc := 0.0;
  for j := 1 step 1 until jmax do begin
    q[1, j] := 1.0;
    numc := numc + w[j] × y[j];
    denc := denc + w[j] end;
  c[2] := numc/denc;
  for j := 1 step 1 until jmax do
    q[2, j] := y[j] - c[2];
  for m := 3 step 1 until mmax do begin
    numc := denc := dend := 0.0;
    for j := 1 step 1 until jmax do begin
      numc := numc + w[j] × y[j] × q[m-1, j] ↑ 2;
      denc := denc + w[j] × q[m-1, j] ↑ 2;
      dend := dend + w[j] × q[m-2, j] ↑ 2 end;
    c[m] := numc/denc; d[m] := denc/dend;
    for j := 1 step 1 until jmax do
```

```
      q[m, j] := (y[j]−c[m]) × q[m−1, j] − d[m] × q[m−2, j] end;
comment evaluate contribution of each orthogonal polynomial
  to the minimization of the residuals;
for n := 1 step 1 until nmax do begin
  denpa[n] := 0.0;
    for i := 1 step 1 until imax do
    denpa[n] := denpa[n] + u[i] × p[n, i] ↑ 2 end;
  for m := 1 step 1 until mmax do begin
    denqa[m] := 0.0;
    for j := 1 step 1 until jmax do
      denqa[m] := denqa[m] + w[j] × q[m, j] ↑ 2 end;
  for n := 1 step 1 until nmax do begin
    for m := 1 step 1 until mmax do begin
      alph := 0.0;
      for i := 1 step 1 until imax do begin
        for j := 1 step 1 until jmax do
          alph := alph + u[i] × w[j] × z[i, j] × p[n, i] × q[m, j]
            end;
    alpha[n, m] := alph/(denpa[n]×denqa[m]);
    beta[n, m] := alpha[n, m] × alph; end end;
comment application of Gauss' criterion to determine the de-
  gree polynomial which yields the closest fit to the given data.
  Gauss' criterion is, strictly speaking, applicable only to cases
  where the weights u[i] and w[j] are unity;
sumzsq := 0.0;
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do
    sumzsq := sumzsq + u[i] × w[j] × z[i, j] ↑ 2 end;
s := t := 1;
for n := 1 step 1 until nmax do begin
  betasum := 0.0;
  for m := 1 step 1 until mmax do begin
    for r := 1 step 1 until n do
      betasum := betasum + beta[r, m];
    if betasum > sumzsq then trialgausscrit := 0.0
    else
    trialgausscrit := (sumzsq−betasum)/(imax×jmax−n×m);
    if n = 1 ∧ m = 1 then gausscrit := trialgausscrit;
    if gausscrit = trialgausscrit then begin
      if n × m < s × t then begin
        s := n;
        t := m end end;
    if gausscrit > trialgausscrit then begin
      gausscrit := trialgausscrit;
      s := n;
      t := m end end end;
nmax := s;
mmax := t;
minsqd := (gausscrit×(imax×jmax−nmax×mmax)/(imax×jmax))
  ↑ ½;
comment evaluation of orthogonal polynomial coefficients;
for n := 1 step 1 until nmax do begin
  pc[n, m] := 1.0;
  for s := 1 step 1 until n − 1 do begin
    pc[n, s] := −a[n] × pc[n−1, s];
    if s ≠ 1 then pc[n, s] := pc[n, s] + pc[n−1, s−1];
    if s ≠ n − 1 then pc[n, s] := pc[n, s] − b[n] × pc[n−2, s]
      end end;
for m := 1 step 1 until mmax do begin
  qc[m, m] := 1.0;
  for t := 1 step 1 until m − 1 do begin
    qc[m, t] := −c[m] × qc[m−1, t];
    if t ≠ then qc[m, t] := qc[m, t] + qc[m−1, t−1];
    if t ≠ m − 1 then qc[m, t] := qc[m, t] − d[m] × qc[m−2, t]
      end end;
comment evaluation of approximating polynomial coefficients;
for s := 1 step 1 until nmax do begin
  for t := 1 step 1 until mmax do begin
    phi[s, t] := 0.0;
    for n := s step 1 until nmax do begin
      for m := t step 1 until mmax do
        phi[s, t] := phi[s, t] + alpha[n, m] × pc[n, s] × qc[m, t]
          end end end;
comment evaluation of dependent variables using the approxi-
  mating polynomial;
minsqdcomp := sumdifcomp := maxidifcomp := 0.0;
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do begin
    zcomp[i, j] := 0.0;
    for s := nmax step − 1 until 1 do begin
      poly := phi[s, mmax];
      for t := mmax − 1 step 1 until 1 do
        poly := poly × y[j] + phi[s, t];
      zcomp[i, j] := zcomp[i, j] × x[i] + poly end;
    rescomp := z[i, j] − zcomp[i, j];
    zcomp[i, j] := zcomp[i, j] + meanz;
    minsqdcomp := minsqdcomp + u[i] × w[j] × rescomp ↑ 2;
    sumdifcomp := sumdifcomp + abs(rescomp);
    if abs (rescomp) > maxdifcomp then
    maxdifcomp := abs(rescomp) end end;
minsqdcomp. := .(minsqdcomp/(imax × jmax) ) ↑ ½;
sumdifcomp := sumdifcomp/(imax × jmax);
end surfacefit
```

CERTIFICATION OF ALGORITHM 164 ORTHOGONAL POLYNOMIAL LEAST SQUARES SURFACE FIT [R. E. Clark, R. N. Kubik, L. P. Phillips, *Comm. ACM*, April 1963]

C. V. Bitterli
Johns Hopkins Univ. Applied Physics Lab., Silver Spring, Md.

The SURFACEFIT algorithm was translated into Fortran and successfully run on an IBM 7094. It was necessary to make the following corrections:

(a) 12th line after

comment evaluate orthogonal polynomials;

should read

numa := *numa* + *u*[*i*] × *x*[*i*] × *p*[*n*−1,*i*] ↑ 2;

(b) 2nd line after

comment evaluation of orthogonal polynomial coefficients;

should read

pc[*n*,*n*] := 1.0;

(c) 12th line after

comment evaluation of orthogonal polynomial coefficients;

should read

if *t* ≠ 1 **then** *qc*[*m*,*t*] := *qc*[*m*,*t*] + *qc*[*m*−1,*t*−1];

(d) 8th line after

comment evaluation of dependent variables using the approximating polynominal

should read

for *t* := *mmax* −1 **step** −1 **until** 1 **do**

The following function was used to generate data for checking this algorithm:

$$z = 1 - x + y - xy + x^2 - y^2$$

for $x = 0, 1, 2, 3, 4$

and $y = 0, 1, 2, 3, 4$

The resulting polynomial was:

$$z = x - 5y - xy + x^2 - y^2$$

which is correct for the normalized variables.

It should be pointed out in the **comment** for this procedure that the resulting polynomial is in the normalized variables and not the original variables.

ALGORITHM 165
COMPLETE ELLIPTIC INTEGRALS

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Reactor Eng. Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

```
procedure KANDE(ml, K, E, tol, alarm);
value ml, tol;
real ml, K, E, tol;
label alarm;
comment this procedure computes the complete elliptic integrals K(ml) = ∫0^π/2 (1 − (1 − ml) sin²ν)^−1/2 dν and E(ml) =
  ∫0^π/2 (1 − (1 − ml) sin²ν)^1/2 dν by the arithmetic-geometric-mean process. The accuracy is limited only by the accuracy of
  the arithmetic.
  Except for the provision of tests for pathological values of the parameter, the calculation of K is only a slight modification of
  the second procedure of Algorithm No. 149 (Comm. ACM. 5 (Dec. 1962), 605). These integrals may also be approximated to
  limited (6D) accuracy by Algorithms 55 and 56 (Comm. ACM. 4 (Apr. 1961), 180). Unless the square-root is exceptionally fast,
  the latter algorithms are probably more efficient for 6D-accuracy.
  The complementary parameter, ml, is chosen as the independent variable, rather than the parameter, m, the modulus,
  k or the modular angle α, because of the possibility of serious loss of significance in generating ml from the other possible
  independent variables when ml is small and dK/dml is very large. These variables are related by ml = 1 − m = 1 − k² =
  cos²α.
  The formal parameter, tol, determines the relative accuracy of the result. To prevent entering a nonterminating loop, tol
  should not be less than twice the relative error in the square root routine. If ml ≦ 0 or if ml > 1, the procedure exits to
  alarm. K(0) = ∞ while E(0) = 1.00000000.
  The body of this procedure has been tested using the Dartmouth SCALP processor for the LGP-30. With tol = 5₁₀ − 7,
  results agreed with tabulated values to within 3 in the seventh significant digit;
begin real a, b, c, sum, temp;
  integer fact;
  if m 1 > 1 ∨ ml ≦ 0 then go to alarm;
  a := fact := 1;
  b := sqrt(ml);
  temp := 1 − ml;
  sum := 0;
iter: sum := sum + temp;
  c := (a − b)/2;
  fact := fact + fact;
  temp := (a + b)/2;
  b := sqrt (a × b);
  a := temp;
  temp := fact × c × c;
  if abs(c) ≧ tol × a ∨ temp > tol × sum then go to iter;
  sum := sum + temp;
  K := 3.141592654/(a + b);
  comment pi must be given to the full accuracy desired;
  E := K × (1 − sum/2)
end
```

CERTIFICATION OF ALGORITHM 165 [S21]
COMPLETE ELLIPTIC INTEGRALS [Henry C. Thacher Jr., *Comm. ACM 6* (Apr. 1963), 163]

I. FARKAS (Recd. 1 Aug. 1968)
Dept. of Computer Science, University of Toronto, Toronto, Ontario, Canada

KEY WORDS AND PHRASES: special functions, complete elliptic integral of the first kind, complete elliptic integral of the second kind
CR CATEGORIES: 5.12

One misprint and one semantic error were found in Algorithm 165:

1. The procedure heading

   procedure *KANDE* (*ml*,*K*,*E*,*tol*,*alarm*);

should read

   procedure *KANDE* (ml,*K*,*E*,*tol*,*alarm*);

2. The second statement in the procedure body

   a := *fact*: = 1;

should read

   fact: = 1; *a*: = 1;

because *fact* and *a* are of different types.

Algorithm 165 was translated into FORTRAN IV on an IBM 7094-II, whose single-precision mantissa has 27 significant bits (about 8 significant decimal digits). Because our *SQRT* program has a relative accuracy of .75₁₀ − 8, *tol* was chosen 3₁₀ − 8. *K* and *E* were generated for ml = (.01(.01)1.0) (to 27 bits) and the results obtained were compared with tables in [1]. For ml = .01 *E* differed by two units in the last place; for all other values of ml, the maximum absolute error was one unit in the last place. The time taken to activate *KANDE* for the above 100 values of ml was 0.1 sec.

REFERENCE:

1. ABRAMOWITZ, M., AND STEGUN, I. A. (Eds.) *Handbook of Mathematical Functions*. NBS Appl. Math. Ser. 55, US Govt. Printing Off., Washington, D. C., 1964.

ALGORITHM 166
MONTECARLO

R. D. RODMAN
Burroughs Corp., Pasadena, Calif.

```
procedure montecarlo (n, a, row, tol, mxm, inv, test, count);
  value n, row, tol, mxm; integer n, row, mxm, count;
  real tol; real array a, inv, test;
  comment this procedure will compute a single row of the
    inverse of a given matrix using a monte carlo technique.
    n is the size of the matrix, array a is the matrix, row indicates
    which inverse row is to be computed, tol is a tolerance factor
    and thus a criterion for terminating the process, mxm is 1000
    times the maximum number of random walks to be taken,
    after which the process is terminated, array inv contains the
    inverse row, array test contains the innerproduct of inv with
    the rowth column of a, count is the number of random walks
    executed upon termination. real procedure RANDOM must
    be declared in the blockhead of procedure MONTE CARLO
    and generates a single random number between 0 and 1. If
    a is the matrix to be inverted, the absolute value of the largest
    eigenvalue of the matrix I − a (I is the unit matrix) must be
    less than one to assure convergence. This procedure is easily
    adapted to finding a single unknown from a set of simultaneous
    linear equations;
  begin integer i, j, k, nwk, lastwalk, walk; real res, p, g;
  real array sum[1:n], v[1:n, 1:n];
start:  p := (n−1)/n × n;
        for i := 1 step 1 until n do for j := 1 step 1 until n do
        v[i,j] := if i ≠ j then −a[i,j]/p else (1−a[i,j])/p;
        nwk := 1000;
        count := res := 0;
        for k := 1 step 1 until n do test [k] := sum [k] := 0;
start1: lastwalk := row; g := 1;
start2: walk := (RANDOM/p) + 1;
        if walk > n then go to stop;
        g := v[lastwalk,walk] × g; lastwalk := walk;
        go to start2;
stop:   count := count + 1; sum[lastwalk] := sum[lastwalk] + g;
        if count < nwk then go to start1;
        for k := 1 step 1 until n do inv[k] := n × sum[k]/count;
        for i := 1 step 1 until n do for k := 1 step 1 until n do
        test[i] := inv[k] × a[k, i] + test[i];
        for i := 1 step 1 until row−1, row+1 step 1 until n do
        res := abs(test[i]) + res; res := abs(test[row]−1) + res;
        if res < tol then go to exit;
        if count ≧ 1000 × mxm then go to exit;
        nwk := nwk + 1000; res := 0;
        for k := 1 step 1 until n do test [k] := 0;
        go to start1;
exit:   end of monte carlo inversion procedure
```

REMARK ON ALGORITHM 166
MONTECARLO INVERSE [R. D. Rodman, *Comm. ACM*, Apr. 1963]

R. D. RODMAN
Burroughs Corp., Pasadena, Calif.

The algorithm contained two errors:

(1) The line which reads

```
start:  p := (n−1)/n × n;
```

should read

```
start:  p := (n−1)/n ↑ 2;
```

(2) The line which reads

```
start2: walk := (random/p) + 1;
```

should read

```
start2: walk: = entier ((random/p) + 1);
```

After making the preceding corrections, procedure montecarlo was transliterated into EXTENDED ALGOL and run successfully on the Burroughs B-5000. Convergence occurred in all cases where the matrix satisfied the conditions set down in the comment statement of the algorithm. It was found that convergence was quickest and the routine most practical for matrices with eigenvalues small relative to one.

ALGORITHM 167
CALCULATION OF CONFLUENT DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS
Institute of Computer Science, University of Toronto, Canada

```
real procedure DVDFC(n, X, V, B, W); integer n;
  real array X, V, B, W;
comment DVDFC ca.culates the forward divided difference
  Δ^n f(X_1, X_2, ··· X_n). n is an integer which takes the values
  n = 1, 2, 3, ··· in turn. X is a real array of dimension at least
  n in which X[i] = X_i for i = 1, 2, ··· , n. The values X_i need
  not be distinct nor in any special order, but once the array X
  is chosen it will fix the interpretation of the arrays B and V.
  If X[1], X[2], ··· , X[n] are in monotonic order, then the effect
  of roundoff upon any nth divided difference is no more than
  would be caused by perturbing each f(X[i]) by n units at most
  in its last significant place. But if the X's are not in mono-
  tonic order, the error can be catastrophic if some of the divided
  differences are relatively large. V is a real array of dimension
  at least n containing the values of the function f(X) and per-
  haps its derivatives at the point X_i. V[i] = f^m(X_i)/m! and
  m = m_i for i = 1, 2, 3, ··· , n. m_i is the number of times that
  the value of X_i has previously appeared in the array X. B is
  a real array of dimension at least n containing backward divided
  differences. Before a reference to DVDFC is executed one should
  have B[i] = Δ^{n-i} f(X_i , X_{i+1} , ··· , X_{n-1}) for i = 1, 2, ··· , n-1.
  After that reference to DVDFC is executed one will find B[i] =
  Δ^{n-i} f(X_i , X_{i+1} , ··· , X_{n-1} , X_n) for i = 1, 2, ··· , n-1, n. When
  n = 1 the initial state of B is irrelevant. W is a real array of
  dimension (2 + m̄) at least, where m̄ is the maximum value of
  m_i for i = 1, 2, ··· , n. W is used for work space;
      begin real DENOM; integer i, j, NK, NIN;
      if n = 1 then go to L1;
      NK := 1;
      for i := 1 step 1 until n do
      begin
      if X[i] = X[n] then begin NK := NK + 1;
          W[NK] := V[i] end
      end i;
      for i := n step -1 until 2 do
      begin W[1] := B[i - 1]; B[i] := W[2];
      NIN := if n - i + 2 < NK then n - i + 2 else NK;
      for j := NIN step -1 until 2 do
      begin
      DENOM := X[n] - X[i + j - 3];
      if DENOM ≠ 0 then go to L2;
      W[j] := W[j + 1];
      if NK - j - 1 ≠ 0 then go Cont;
      NK := NK - 1;
      go to Cont;
L2:   W[j] := (W[j] - W[j - 1])/DENOM;
Cont: end j
      end i;
      B[1] := W[2];
      go to L3;
L1:   B[1] := V[1];
L3:   DVDFC := B[1]
      end DVDFC
```

The following program segment is an example of how *DVDFC* can be used to construct a table of forward or backward differences.

```
for n := 1 step 1 until N do
begin
X[n] := ··· ; V[n] := ··· ; F[n] := DVDFC(n, X, V, B, W)
  end;
```

The array F can be used in *FNEWT*(z, N, X, F, R, D, E) or the array B in *BNEWT*(z, N, X, B, P, D, E). See algorithms "Newton interpolation with forward (backward) divided differences."

DVDFC has been written as a FORTRAN II function and is available from I.C.S., University of Toronto;

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NEWTON INTERPOLATION WITH BACKWARD DIVIDED DIFFERENCES [W. Kahan and I. Farkas, *Comm. ACM*, Apr. 1963]
CERTIFICATION OF ALGORITHM 169
NEWTON INTERPOLATION WITH FORWARD DIVIDED DIFFERENCES [W. Kahan and I. Farkas, *Comm. ACM*, Apr. 1963.]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

The bodies of these procedures were tested on the LGP-30 computer using the Dartmouth SCALP compiler. Compilation and execution revealed no syntactical or mathematical errors.

It is to be noted that, although with Algorithm 169, reducing the value of N from that used to generate F leads to an interpolation polynomial based on fewer points, this is not true for Algorithm 168. This flexibility could be supplied by adding an additional formal parameter, *deg*, say, to the procedure, and by making the **for** statement read:

"**for** i := N − *deg* **step** 1 **until** N **do** ··· "

The logic of the error estimate in Algorithms 168 and 169 is not entirely clear. However, it appears that the estimate can be adjusted for different precision of arithmetic by adjusting the constant $3_{10}-8$ appropriately. For the SCALP arithmetic, this constant was changed to $1_{10}-7$.

The algorithms were tested on the examples given by Milne-Thomson [*The Calculus of Finite Differences*, p. 4, Macmillan, 1951] and by Milne [*Numerical Calculus*, p. 204, Princeton, 1949]. In both examples, Algorithm 167 reproduced the divided difference table, and both Algorithms 168 and 169 reproduced the input values. As a check of the calculation of confluent divided differences, values of the exponential function of its first two derivatives at $x = 5.0$ and 6.0 were used. The difference table shown in Table A was obtained.

* Work supported by the U. S. Atomic Energy Commission.

TABLE A

n	$X[n]$	$V[n]$	$B[n]$	$B[n-1]$	$B[n-2]$	$B[n-3]$	$B[n-4]$	$B[n-5]$
1	5.0	148.4132	148.4132					
2	5.0	148.4132	148.4132	148.4132				
3	6.0	403.4288	403.4287	255.0155	106.6023			
4	6.0	403.4288	403.4287	403.4287	148.4132	41.81091		
5	5.0	74.20658	148.4132	255.0155	148.4132	41.81091	9.415191	
6	6.0	201.7144	403.4287	255.0155	148.4132	53.30115	11.49023	2.075043

The forward differences lie along the top diagonal.
Use of these results with *BNEWT* and with *FNEWT* gave the following results, for $N = 6$.

z	*BNEWT*			*FNEWT*		
	P	D	E	R	D	E
5.000000	148.4132	148.4132	$.4567298 \times 10^{-4}$	148.4132	148.4132	$.7420658 \times 10^{-5}$
5.500000	244.6973	244.6924	$.4173722 \times 10^{-4}$	244.6973	244.6924	$.3078276 \times 10^{-4}$
6.000000	403.4287	403.4287	$.2017143 \times 10^{-4}$	403.4287	403.4287	$.7441404 \times 10^{-4}$

ALGORITHM 168
NEWTON INTERPOLATION WITH BACKWARD DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS
Institute of Computer Science, University of Toronto, Canada

```
procedure BNEWT(z, N, X, B, P, D, E); value z, N;
  real z, P, D, E; integer N; real array X, B;
comment X is a real array of dimension at least N in which
  X[i] = X_i for i = 1, 2, 3, ··· , N. The values X_i need not be
  distinct nor in any special order, but once the array X is chosen
  it will fix the interpretation of the array B. B is a real array of
  dimension at least N and contains the backward divided differ-
  ences B[i] = Δf(X_i , X_{i+1} , ··· , X_N)  i = 1, 2, ··· , N. If two
  or more of the values X_i are equal then some of the B's must
  be confluent divided differences, see algorithm: "Calculation of
  confluent divided differences." P is the value of the following
  polynomial in z of degree N−1 at most, B(N) + (z−X_N)·
  {B(N−1) + (z−X_{N−1}){B(N−2) + ··· + (z−X_2)B(1)} ··· }}.
  This polynomial is an interpolation polynomial which would,
  but for rounding errors, match values of the function f(x) and
  any of its derivatives that DVDFC might have been given. D
  is the value of the derivative of P. E is the maximum error in
  P caused by roundoff during the execution of BNEWT. The
  error estimate is based upon the assumption that the result of
  each floating point arithmetic operation is truncated to 27 sig-
  nificant binary digits as is the case in FORTRAN programs on
  the 7090. BNEWT has been written as a FORTRAN II subroutine
  and is available from I.C.S., University of Toronto;
begin real z1; integer i;
P := D := E := 0;
for i := 1 step 1 until N do
begin
z1 := z − X[i];
D := P + z1 × D;
P := B[i] + z1 × P;
E := abs(P) + E × abs(z1)
end;
E := (1.5×E − abs(P))×3_10 − 8
end BNEWT
```

The bodies of these procedures were tested on the LGP-30 computer using the Dartmouth SCALP compiler. Compilation and execution revealed no syntactical or mathematical errors.

It is to be noted that, although with Algorithm 169, reducing the value of N from that used to generate F leads to an interpolation polynomial based on fewer points, this is not true for Algorithm 168. This flexibility could be supplied by adding an additional formal parameter, *deg*, say, to the procedure, and by making the **for** statement read:

"**for** $i := N -$ *deg* **step** 1 **until** N **do** ··· "

The logic of the error estimate in Algorithms 168 and 169 is not entirely clear. However, it appears that the estimate can be adjusted for different precision of arithmetic by adjusting the constant $3_{10}-8$ appropriately. For the SCALP arithmetic, this constant was changed to $1_{10}-7$.

The algorithms were tested on the examples given by Milne-Thomson [*The Calculus of Finite Differences*, p. 4, Macmillan, 1951] and by Milne [*Numerical Calculus*, p. 204, Princeton, 1949]. In both examples, Algorithm 167 reproduced the divided difference table, and both Algorithms 168 and 169 reproduced the input values. As a check of the calculation of confluent divided differences, values of the exponential function of its first two derivatives at $x = 5.0$ and 6.0 were used. The difference table shown in Table A was obtained.

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HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

TABLE A

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The forward differences lie along the top diagonal.
Use of these results with *BNEWT* and with *FNEWT* gave the following results, for $N = 6$.

z	*BNEWT*			*FNEWT*		
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ALGORITHM 169
NEWTON INTERPOLATION WITH FORWARD DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS
Institute of Computer Science, University of Toronto, Canada

```
procedure FNEWT(z, N, X, F, R, D, E); value z, N;
  real z, R, D, E; integer N; real array X, F;
comment X is a real array of dimension at least N in which
  X[i] = X_i for i = 1, 2, ··· , N. The values X_i need not be
  distinct nor in any special order, but once the array X is
  chosen it will fix the interpretation of the array F. F is a
  real array of dimension at least N and contains the forward
  divided differences F[i] = Δf(X_1 , X_2 , ··· , X_i)  i = 1, 2, ··· , N. If
  two or more of the values X_i are equal then some of the F's
  must be confluent divided differences, see algorithm: "Calcu-
  lation of confluent divided differences." R is the value of the fol-
  lowing polynomial in z of degree N-1 at most, F(1) + (z-X_1)·
  {F(2) + (z-X_2){F(3) + ··· + (z-X_{N-1})F(N)} ··· }. This
  polynomial is an interpolation polynomial which would, but
  for rounding errors, match values of the function f(x) and any
  of its derivatives that DVDFC might have been given. D is the
  value of the derivative of R. E is the maximum error in R
  caused by roundoff during the execution of FNEWT. The
  error estimate is based upon the assumption that the result of
  each floating-point arithmetic operation is truncated to 27
  significant binary digits as is the case in FORTRAN programs
  on the 7090. FNEWT has been written as a FORTRAN II sub-
  routine and is available from I.C.S., University of Toronto;
begin real z1; integer i;
R := D := E := 0;
for i := N step -1 until 1 do
begin
z1 := z - X[i];
D := R + z1 × D;
R := F[i] + z1×R;
E := abs(R) + abs(z1)×E
end;
E := (1.5×E - abs(R))×3_10 - 8
end FNEWT
```

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TABLE A

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The forward differences lie along the top diagonal.

Use of these results with *BNEWT* and with *FNEWT* gave the following results, for $N = 6$.

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6.000000	403.4287	403.4287	$.2017143 \times 10^{-4}$	403.4287	403.4287	$.7441404 \times 10^{-4}$

ALGORITHM 170
REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS

PAUL E. HENNION
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```
real procedure POLYMATRIX (A, NCOL, N, COE, NP1);
  value A, NCOL, N; real array A; integer NCOL, N;
comment this procedure will expand a general determinant,
  where each of the elements are polynomials in the Laplace
  complex variable. This program is useful for the investigation of
  dynamic stability problems when using the transfer function
  approach. The process is one of triangularization of a poly-
  nomial matrix with real coefficients whereupon multiplication
  of the diagonal elements the determinant polynomial is formed.
  The polynomial matrix as defined herein is a matrix whose
  elements are polynomials of the form ∑(i=0..N) a_i x^i. When such a
  matrix is triangularized, all elements below the main diagonal
  are nulled. Then upon expanding, the nonvanishing terms are
  those formed by the product of these diagonal elements. Hence
  stability criteria may be checked by evaluating the roots of the
  characteristic equation thus formed using some suitable root
  extracting routine.

  Consider the polynomial matrix with quadratic elements
  (N = 2). In this case the three-dimensional input matrix A is
  size A[1:NCOL, 1:NCOL, 1:M], where NCOL is the order of
  the matrix and M = N × NCOL + 1. Here the first subscript
  of A refers to the row, the second to the column, and the third
  to the polynomial coefficient. Therefore, prior to entry the con-
  stant term of a general polynomial element is contained in
  A[i, j, 1], the linear term is contained in A[i, j, 2], and the
  quadratic term in A[i, j, 3]. Upon completion of the routine, the
  coefficients of the determinant polynomial are contained in
  COE [1:M]. The constant coefficient being in COE [1], the linear
  coefficient in COE [2], the quadratic coefficient in COE [3], etc.
  The variable NP1 will specify the number of coefficients of the
  determinant polynomial. In general NP1 ≠ M since some terms
  may vanish during the expansion.

  If the polynomials comprising the matrix elements are not
  all of equal degree, set N prior to entry equal to the degree of
  the highest ordered polynomial;
begin real sa, sb; integer i, j, k, j1, j2, j3, j4, j5, j6, j7, j8, j9, j10,
  j11, NP1, M; array C1[1:M], C2[1:M], COE[1:M];
  integer array MAT [1:NCOL, 1:NCOL];
start: M := N×NCOL+1; for i := 1 step until NCOL do
  begin for j := 1 step 1 until NCOL do begin MAT [i,j] := 0;
  for k := 1 step 1 until M do begin
  if A[i, j, k]≠0 then MAT [i, j] := k; end end end; j1 := 1;
L0: j9 := 0; for i := j1 step 1 until NCOL do begin
  if MAT [i,j1]<0 then go to exit;
  else if MAT [i, j1] =0 then go to L1
  else j9 := j9+1; j3 := i;
L1: end; if (j9−1)<0 then go to exit
  else if (j9−1)>0 then go to L2
  else if (j3−j1)<0 then go to exit
  else if (j3−j1)=0 then go to L12
  else for j := j1 step 1 until NCOL do
  begin j2 := MAX(MAT [j3,j], MAT [j1,j]); j4 := MAT [j3,j];
  MAT [j3,j] := MAT [j1, j]; MAT [j1,j] := j4;
  for k := 1 step 1 until j2 do
  begin sa := A [j3, j,k]; A[j3,j,k] := A[j1, j, k];
  A[j1,j,k] := −sa; end end; go to L12;
L2: j3 := j1+1; for i := j3 step 1 until NCOL do begin
L3: if (MAT[i,j1])<0 then go to exit
  else if [MAT [i,j1])=0 then go to L11
  else if (MAT [j1,j1])<0 then go to exit
  else if (MAT[j1,j1])=0 then go to L4
  else if (MAT [i,j1] −MAT [j1,j1]) ≧ 0 then go to L5 else
L4: for j := j1 step 1 until NCOL do begin
  j2 := MAX(MAT [j1,j], MAT [i, j]); j4 := MAT [j1,j];
  MAT (j1,j] := MAT [i,j]; MAT [i,j] := j4;
  for k := 1 step 1 until j2 do begin sa := A[i,j,k];
  A[i,j,k] := A[j1,j,k]; A[j1,j,k] := −sa;
  end end; go to L3;
  comment Interchange row i with j1;
L5: j7 := MAT [i,j1]; j5 := MAT [j1,j1]; j6 := j7−j5;
  sb := A[i,j1,j7]/A[j1,j1,j5];
  if (abs(sb)−4)<0 then go to L6
  else if (j6)<0 then go to exit
  else if (j6)=0 then go to L4 else
L6: for j := j1 step 1 until NCOL do begin j5 := MAT [j1, j];
  for k := 1 step 1 until j5 do begin j7 := k+j6;
  if (j7−M)>0 then go to L10 else
L7: if (abs(A[i,j,j7] −sb×A[j1,j,k])−2₁₀−8)≦0 then go to L8
  else A[i,j,j7] := A[i,j,j7] −sb×A[j1,j,k];
  go to L9;
L8: A[i,j,j7] := 0;
L9: end end;
L10: for j := j1 step 1 until NCOL do begin
  j7 := MAX(MAT [i,j], MAT[j1,j]+j6); MAT [i,j] := 0;
  for k := 1 step 1 until M do begin if (A[i,j,k])≠0 then
  MAT [i,j] := k end end;
L11: end; go to L0;
L12: j1 := j1+1; if (j1−NCOL)<0 then go to L0 else
  for j := 1 step 1 until NCOL do begin
  j2 := MAT [j,j];
  for k := 1 step 1 until j2 do C1[k] := A[j,j,k];
L13: if (j−1)<0 then go to exit
  else if (j−1)=0 then go to L14
  else for k := 1 step 1 until NP1 do C2[k] := COE[k];
  for k := 1 step 1 until M do COE[k] := 0;
  if (j2)<0 then go to exit
  else if (j2)=0 then go to L15
  else for k := 1 step 1 until j2 do begin
  for j10 := 1 step 1 until NP1 do begin
  j11 := k+j10−1;
  COE[j11]:=COE[j11]+C1[k]×C2[j10];
  end end; NP1 := j11; go to L15;
L14: for k := 1 step 1 until j2 do COE [k] := C1 [k];
  NP1 := j2;
L15: end;
exit: end POLYMATRIX
```

REMARK ON ALGORITHM 170
REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS [P. E. Hennion, *Comm. ACM*, Apr. 1963]

P. E. HENNION
Giannini Controls Corp., Berwyn, Penn.

Four typographical errors were found upon reviewing the procedure. The following corrections should be made:

(1) The increment for the **for** statement of line start:, should be 1.
(2) The colon at the end of the third line after line start:, should be replaced by a semicolon.
(3) The semicolon at the end of the first line after line *LO*:, may be removed.
(4) The last statement of the first column should read:

$$MAT[i,j] := k; \textbf{ end end};$$

CERTIFICATION OF ALGORITHM 170 [F3]
REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS [P. E. Hennion, *Comm. ACM* 6 (April 1963), 165; 6 (Aug. 1963), 450]

KAREN B. PRIEBE (Recd. 18 Dec. 1963 and 18 Feb. 1964)
Woodward Governor Co., Rockford, Ill.

Algorithm 170 was translated into FAST for the NCR 315 and gave satisfactory results with the following corrections:

1. **real procedure** ... **integer** *NCOL*, *N*; should be replaced by

```
procedure POLYMATRIX (A, NCOL, N, COE, NP1);
  value NCOL, N; real array A, COE;
  integer NCOL, N, NP1;
```

2. At the end of the first comment add:

The global integer procedure *MAX* is assumed and furnishes the maximum of two integers.

3. **integer** *i*, *j*, *k*, ... *COE*[1:*M*];

should be replaced by

```
integer i, j, k, j1, j2, j3, j4, j5, j6, j7, j8, j9, j10, j11, M;
array C1, C2[1:N×NCOL+1];
```

4. Immediately after *start*: the statement

$$NP1 := N + 1;$$

should be added, and the third line after *start*: i.e.,

for *k* := 1 **step** 1 **until** *M* **do begin**

should be replaced by

for *k* := 1 **step** 1 **until** *NP*1 **do begin**

5. The third line after *L*10: i.e.,

for *k* := 1 **step** 1 **until** *M* **do** ...

should be replaced by

for *k* := 1 **step** 1 **until** *j7* **do** ...

The last two changes simply shorten both of the indicated FOR statements.

[EDITOR'S NOTE. In addition to the above corrections, we have two comments on the Remark on Algorithm 170 by Hennion, *loc. cit.*, p. 450:

First, the semicolon at the end of the first line after *L*0 MUST be removed.

Second, correction (4) is irrelevant.

The referee confirms that a transcription into Burroughs Extended ALGOL of the program as corrected by Mrs. Priebe runs on the B5000.—G.E.F.]

Note. There is no algorithm for the number 171.
Inadvertently this number was never assigned.

Note. There is no algorithm for the number 172.
Inadvertently this number was never assigned.

ALGORITHM 173
ASSIGN

OTOMAR HÁJEK
Research Institute of Mathematical Machines, Prague, Czechoslovakia

```
procedure assign (a) the value of : (b) with dimension : (dim)
  indices : (ind) bounds : (low, up) tracer : (j);
value dim; integer dim, ind, low, up, j;
comment This procedure uses Jensen's device (cf. ALGOL
  Report, procedure Innerproduct) twice: the a, b may depend on
  ind and also ind, low, up may depend on j;
begin
  j := dim;
  for ind := low step 1 until up do
    if dim > 1
    then
      begin
        assign (a, b, dim-1, ind, low, up, j);
        j := dim
      end
    else a := b
end assign;
comment The obvious use of "assign" is in assigning the value
  of one array to another. The point here is that one procedure
  declaration serves for all the dimensions used. In fact, the
  dimension may even be a variable: thus a procedure essentially
  identical with "assign" was used by the author in implementing
  the recursive own process in an ALGOL compiler.
    However, in addition to this, "assign" can have further
  functions, as illustrated below. The activation assign (a, (if
  i=1 then false else a) ∨ b[i,i], 1, i, 1, n, j) will calculate the
  join-trace of a Boolean 2-dimensional array b.
  assign (a[i1,i2], (if i3=1 then 0 else a[i1,i2]) + b[i1,i3] × c[i3,i2],
    3, ij, 1, if j = 1 then n else if j = 2 then m else p, j)
  will assign to a the matrix product of b, c. It may be noticed that,
  more generally, "assign" will perform all the tensor operations,
  e.g. tensor multiplication, alternation, etc.
```

CERTIFICATION OF ALGORITHM 173
ASSIGN [Otomar Hájek, *Comm. ACM*, June 1963]

R. S. SCOWEN
English Electric Co. Ltd., Whetstone, Leicester, England

Algorithm 173 (ASSIGN) has been tested successfully using the DEUCE ALGOL 60 compiler. The only changes necessary were the addition of specifications for the formal parameters *a*, *b* (DEUCE ALGOL 60 compiler requires specifications for all formal parameters).

The author's example, *assign* (*a*[*i*[1], *i*[2]], (**if** *i*[3]=1 **then** 0.0 **else** *a*[*i*[1], *i*[2]]) + *b*[*i*[1], *i*[3]] × *c*[*i*[3], *i*[2]], 3, *i*[*j*], 1, **if** *j* = 1 **then** *n* **else if** *j* = 2 **then** *m* **else** *p*, *j*);
did form the matrix product $B \times C$ and store it in A.

The algorithm was also used to read a matrix into the computer using the procedure call

```
assign (b[i[1], i[2]], read, 2, i[j], 1,
  if j = 1 then n else p, j);
```

(*read* is a real procedure which takes the value given by the next number on the input tape).

These examples took about three times as long to run as the simpler equivalent statements

```
for i := 1 step 1 until n do
for j := 1 step 1 until m do
begin
  a[i, j] := 0.0;
  for k := 1 step 1 until p do
  a[i, j] := a[i, j] + b[i, k] × c[k, j]
end;
```

and

```
for j := 1 step 1 until p do
for i := 1 step 1 until n do
b[i, j] := read;
```

CERTIFICATION OF ALGORITHM 173
ASSIGN [O. Hájek, *Comm. ACM*, July 1963]

Z. FILSAK and L. VRCHOVECKÁ
Research Institute of Mathematical Machines, Prague, and Computing Center Kancelářské stroje, Prague

The algorithm was modified for input to the Elliott-ALGOL system as follows. In Elliott-ALGOL, name-called parameters in recursive procedures are prescribed. Luckily, the only parameter which varies during the recursive call in the body of *Assign* is called by value (it is the parameter *dim* which determines depth of recursion). The body of *Assign* was replaced by (i) a procedure declaration *Ass*(*dim*), whose body is that of the original *Assign*, but with the recursive call of *Assign* replaced by that of *Ass*, and (ii) a single statement, the activation of *Ass*(*dim*).

The resulting procedure was tested (on the National-Elliott 803 in the Computing Center), on a rather large set of examples, including those described in the text following Algorithm 173. It was found that in the last example, matrix multiplication, indices i_1 and i_3 should be interchanged throughout.

No changes of the algorithm itself were necessary. It seems that the modification described above, motivated by limitations of Elliott-ALGOL, also improve efficiency, at least for large dimensions of the arrays concerned.

ALGORITHM 174
A POSTERIORI BOUNDS ON A ZERO OF A POLYNOMIAL*

ALLAN GIBB
University of Alberta, Calgary, Alberta, Canada

```
comment The procedures below make use of Algorithm 61, Procedures for Range Arithmetic [Comm. ACM 4 (1961)]. It is assumed that the procedures below and the range arithmetic procedures are contained in an outer block and, therefore, that the procedures are available as required. Together the procedures make possible an attempt to determine absolute bounds on a zero of a polynomial given an initial estimate of the zero. The procedures below are given for the complex case but may readily be adapted for the real case;
procedure RngPlyC (N, A, Z, P);
comment RngPlyC finds bounds [P1, P2] + i[P3, P4] on the value of an nth degree polynomial Σ_{k=0}^{n} {[a_{4k+1}, a_{4k+2}] + i[a_{4k+3}, a_{4k+4}]}z^k with complex range coefficients for a complex range argument z = [Z1, Z2] + i[Z3, Z4];
integer N; array A, Z, P;
begin integer K, J; array X, Y[1 : 4];
P[1] := P[2] := P[3] := P[4] := 0;
for K := 4 × N step −4 until 0 do
  begin for J := 1 step 1 until 4 do X[J] := A[K+J];
  RNGMPYC (P[1], P[2], P[3], P[4], Z[1], Z[2], Z[3], Z[4], Y[1],
           Y[2], Y[3], Y[4]);
  RNGSUMC (Y[1], Y[2], Y[3], Y[4], X[1], X[2], X[3], X[4],
           P[1], P[2], P[3], P[4])
  end
end;
procedure RngAbsC (A, C);
comment RngAbsC produces the range absolute value [C1, C2] of the complex range number [A1, A2] + i[A3, A4];
array A, C;
begin array B[1 : 4];
RANGESQR (A[1], A[2], B[1], B[2]);
RANGESQR (A[3], A[4], B[3], B[4]);
RANGESUM (B[1], B[2], B[3], B[4], C[1], C[2]);
C[1] := sqrt(C[1]);
C[2] := sqrt(C[2]);
comment It is assumed that the accuracy of the sqrt routine used is known and that the maximum error in sqrt(C) is ± K × CORRECTION(C). K is to be replaced below by its appropriate numerical value;
C[1] := C[1] − K × CORRECTION (C[1]);
C[2] := C[2] + K × CORRECTION (C[2])
end;
procedure BndZrPlyC (N, ZOR, ZOJ, A, W,);
integer N; real ZOR, ZOJ; array A, W;
comment BndZrPlyC attempts to determine bounds [W1, W2] + i[W3, W4] on a zero of an N-th degree polynomial in z with complex range coefficients. It is assumed that an estimate ZO = ZOR + iZOJ of the zero is available. The following theorem is used. Assume f is regular at z0 with f'(z0) ≠ 0. Let h0 = −f(z0)/f'(z0), let Δ be the region | z − z0 | ≦ r | h0 |, and assume that f is regular in Δ. If, for some r > 0, | f'(z) | ≧ (1/r). | f'(z0) | for all z ∈ Δ then Δ contains a zero of f (see [1], pp. 29–31);
begin integer I, J; array B[1:4×N], E, F, FP, D[1:4], AF, AFP, G[1:2];
real RH, RHS, NL, NR, R, RNL, RNR;
for I := 1 step 1 until N do
  begin J := 4 × I;
  RANGEMPY (I, I, A[J+1], A[J+2], B[J−3], B[J−2]);
  RANGEMPY (I, I, A[J+3], A[J+4], B[J−1], B[J])
  end;
E[1] := E[2] := ZOR; E[3] := E[4] := ZOJ;
RngPlyC(N, A, E, F);
RngAbsC(F, AF);
RngPlyC(N−1, B, E, FP);
RngAbsC(FP, AFP);
RANGEDVD(AF[1], AF[2], AFP[1], AFP[2], NL, NR);
R := 2;
1: RANGEMPY(R, R, NR, NR, RNL, RNR);
RANGESUM(ZOR, ZOR, −RNR, RNR, W[1], W[2]);
RANGESUM(ZOJ, ZOJ, −RNR, RNR, W[3], W[4]);
comment We have replaced the disk of the theorem by a square;
RngRlyC(N−1, B, W, D);
RngAbsC(D, G);
if G[1] = 0 then go to failure1;
comment failure1 and failure2 are non-local labels;
RANGEDVD(AFP[2], AFP[2], R, R, RH, RHS);
if G[1] < RHS then
  begin R := 2 × R;
  if R > 1024 then go to failure2;
  go to 1
  end
end

comment The following procedure may replace BndZrPlyC above;
procedure BndZrPlyC2 (N, ZOR, ZOJ, A, W);
integer N; array A, W; real ZOR, ZOJ;
comment BndZrPlyC2 is similar to BndZrPlyC above. The theorem used here follows. If, in the disk | z − z0 | ≦ 2 | h0 | we have | f''(z) | ≦ | f'(z0) |/(2 | h0 |), then there is a unique zero in the disk (see [2, pp. 43-50];
begin integer I, J; array B[1:4×N], C[1:4×N−4], F, D, P, S[1:4], X, T, Q, Y[1:2]; real V, VP, R, RL;
for I := 1 step 1 until N do
  begin J := 4 × I;
  RANGEMPY(I, I, A[J+1], A[J+2], B[J−3], B[J−2]);
  RANGEMPY(I, I, A[J+3], A[J+4], B[J−1], B[J])
  end;
for I := 1 step 1 until N − 1 do
  begin J := 4 × I;
  RANGEMPY(I, I, B[J+1], B[J+2], C[J−3], C[J−2]),
  RANGEMPY(I, I, B[J+3], B[J+4], C[J−1], C[J])
  end;
D[1] := D[2] := ZOR;
D[3] := D[4] := ZOJ;
RngPlyC(N, A, D, F);
RngPlyC(N−1, B, D, P);
RngAbsC(F, T);
RngAbsC(P, X);
if X[1] = 0 then go to failure1;
```

* These procedures were developed under Office of Naval Research Contract Nonr-225(37) at Stanford University. The author wishes to thank Professor George E. Forsythe for assistance with this work.

```
comment failure1 and failure2 are non-local labels;
RANGEDVD(T[1], T[2], X[1], X[2], Q[1], Q[2]);
RANGEMPY(2, 2, Q[2], Q[2], RL, R);
RNGSUMC(-R, R, -R, R, ZOR, ZOR, ZOJ, ZOJ, W[1], W[2],
  W[3], W[4]);
RngPlyC(N - 2, C, W, S);
RngAbsC(S, Y);
RANGEDVD(X[1], X[1], R, R, V, VP);
if Y[2] > V then go to failure2
end
```

References:
1. GIBB, ALLAN. ALGOL procedures for range arithmetic. Tech. Report No. 15, Appl. Math. and Statistics Laboratories, Stanford University (1961).
2. OSTROWSKI, A. M. *Solution of equations and systems of equations*. Academic Press, New York, 1960.

ALGORITHM 175
SHUTTLE SORT

C. J. SHAW AND T. N. TRIMBLE
System Development Corporation, Santa Monica, Calif.

```
procedure shuttle sort (m, Temporary, N);
value m; integer m; array N[1:m];
comment This procedure sorts the list of numbers N[1] through
  N[m] into numeric order, by exchanging out-of-order number
  pairs. The procedure is simple, requires only Temporary as
  extra storage, and is quite fast for short lists (say 25 numbers)
  and fairly fast for slightly longer lists (say 100 numbers). For
  still longer lists, though, other methods are much swifter. The
  actual parameters for Temporary and N should, of course, be
  similar in type;
  begin integer i, j;
  for i := 1 step 1 until m - 1 do
    begin
    for j := i step -1 until 1 do
      begin
      if N[j] ≤ N[j+1] then go to Test;
Exchange: Temporary := N[j]; N[j] := N[j+1];
          N[j+1] := Temporary; end of j loop;
Test: end of i loop
  end shuttle sort
```

CERTIFICATION OF ALGORITHM 175
SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm. ACM*, June 1963]

GEORGE R. SCHUBERT*
University of Dayton, Dayton, Ohio
* Undergraduate research project, Computer Science Program, Univ. of Dayton.

Algorithm 175 was translated into BALGOL and ran successfully on the Burroughs 220. The following actual sorting times were observed:

Number of Items	*Average Time* (sec)
25	1.6
50	6.2
100	25.8
250	181
500	684

The algorithm can be extended so that the sort is made on one array, while retaining a one-to-one correspondence to a second array. This is done by inserting immediately before **end** of the j loop the following:

Temporary := $Y[j]$; $Y[j]$:= $Y[j+1]$; $Y[j+1]$:= *Temporary*; where $Y[k]$ is the element to be associated with $N[k]$. Other variations are obviously possible.

REMARK ON ALGORITHM 175
SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm. ACM 6*, June 1963]

O. C. JUELICH
North American Aviation, Inc., Columbus, Ohio

The authors of this algorithm do well to remind the reader that "Shuttle Sort" is not an efficient procedure, except for lists of items so short that they do not justify the housekeeping apparatus needed by the usual sorting routines.

The algorithm as published is not free from errors. The statement

for $j := i$ **step** -1 **until** 1 **do**

should be replaced by either:

for $j := m - 1$ **step** -1 **until** i **do**

or

for $j := 1$ **step** 1 **until** $m - i$ **do**

In the former case the process can be visualized as placing the ith smallest element in place on the ith pass; in the latter the ith largest element is put in place on the ith pass.

The label "*Test*" should precede the delimiter "**end** of j loop" rather than the "**end** of i loop". The algorithm can be slightly accelerated by rewriting the body of the procedure·

```
begin integer i, j, j max;
  i := m - 1;
loop: j max := 1;
  for j := 1 step 1 until i do
    begin
    compare: if N[j] > N[j + 1] then
      begin Exchange: Temporary := N[j];
        N[j] := N[j + 1];
        N[j + 1] := Temporary;
        j max := j
      end Exchange;
    end of j loop;
  i := j max;
  if i > 1 then go to loop;
end shuttle sort
```

The revised procedure body will eliminate redundant iterations when some of the data is already ordered.

It was studied in this form by R. L. Boyell and the writer on the ORDVAC at Ballistics Research Laboratories, Aberdeen Proving Ground, in 1955. For randomly ordered data the i-loop may be expected to be executed about $m-\sqrt{m}$ times.

REMARK ON ALGORITHM 175
SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm. ACM 6* (June 1963), 312; G. R. Schubert, *Comm. ACM 6* (Oct. 1963), 619; O. C. Juelich, *Comm. ACM 6* (Dec. 1963), 739]

OTTO C. JUELICH (Recd. 18 Dec. 1963)
North American Aviation, 4300 E. Fifth Ave., Columbus, Ohio

The appearance of Schubert's certification has caused me to restudy the algorithm. What I supposed were errors amount to a rearrangement of the order in which the comparisons are carried

out. The efficiency of the algorithm is not much affected by the rearrangement, since the number of executions of the statements labeled *Exchange* remains the same.

ALGORITHM 176
LEAST SQUARES SURFACE FIT
T. D. ARTHURS
The Boeing Company, Transport Division, Renton, Wash.

```
procedure SURFIT (F, z, W, m, n) answers: (a, e, rms);
integer m, n; real rms; array F, z, W, e;
procedure Invert, sqrt;
comment Given a set of m ordinates and the corresponding
  values of n prescribed general functions, (f_i), of one or more
  linearly independent variables, this procedure fits the points,
  in the least squares sense, with a function of the form a_1f_1 + a_2f_2
  + . . . + a_nf_n where a_i are the unknown coefficients. Also com-
  puted are the vectors of residuals (e_j) and their lengths (rms).
  Provision is made for weighting the data points. Essentially, the
  matrix equation F^T WFa = F^T Wz is solved, where a is the vector
  of unknowns, W is an m × m diagonal matrix of data point
  weights, z is the vector of ordinate values and F is the
  m × n matrix of corresponding function values. The availa-
  bility of a procedure Invert, which replaces a real matrix with
  its inverse, is assumed;
begin integer i, j, k; real sqsum, g; array G[1:n, 1:n];
  comment G is working space for the inversion procedure;
  sqsum := 0;
  for i := 1 step 1 until n do
  for j := 1 step 1 until n do
  begin G[i, j] := 0;
    for k := 1 step 1 until m do
    G[i, j] := G[i, j] + F[k, i] × F[k, j] × W[k]
  end j;
  Invert (G, n);
  for i := 1 step 1 until n do
  begin a[i] := 0;
    for j := 1 step 1 until m do
    begin g := 0;
      for k := 1 step 1 until n do
      g := g + G[i, k] × F[j, k];
      a[i] := a[i] + g × z[j] × W[j]
    end j
  end i;
  for i := 1 step 1 until m do
  begin e[i] = y[i];
    for j := 1 step 1 until n do
    e[i] := e[i] − a[j] × F[i, j];
    sqsum := sqsum + e[i] ↑ 2
  end i;
  rms := sqrt (sqsum/m)
end SURFIT
```

Remark on Algorithm 176 [E2]
Least Squares Surface Fit [T.D. Arthurs, *Comm. ACM 6* (June 1963), 313]

Ernst Schuegraf [Recd. 1 Mar. 1971]
Department of Mathematics. St. Francis Xavier University, Antigonish, Nova Scotia, Canada

Algorithm 176 contains one misprint. The line which reads:
begin $e[i] = y[i]$;
should read:
begin $e[i] = z[i]$;

ALGORITHM 177
LEAST SQUARES SOLUTION WITH CONSTRAINTS

M. J. SYNGE
The Boeing Company, Transport Division, Renton, Wash.

```
procedure CONLSQ (A, y, w, n, m, r) results: (x) residuals:
  (e, rms);
real rms; integer n, m, r; array A, y, w, x, e; procedure
  abs, SURFIT;
comment This procedure solves an overdetermined set of n
  simultaneous linear equations in m unknowns, Ax = y. The
  first r equations (r≤m) are satisfied exactly and the remaining
  n − r are satisfied as well as possible by the method of least
  squares. Each equation is assigned a weight from the vector w,
  although the first r weights have no relevance. This procedure
  may be used for curve or surface fitting when the approximating
  function or its derivatives are required to have fixed values at a
  number of points;
begin integer i, j, k, ii, ick; integer array ic[1:m];
  array B[1:n−r, 1:m−r]; real Amax;
  for i := 1 step 1 until r do
  begin k := 1; for j := 2 step 1 until m do
    begin if abs (A[i, j]) > abs (A[i, k]) then k := j; end;
    ic[i] := k; Amax := A[i, k]; for j := 1 step 1 until m do
    A[i, j] := A[i, j]/Amax; y[i] := y[i]/Amax;
    for ii := 1 step 1 until r do
    begin if ii = i then go to skip; Amax := A[ii, k];
      for j := 1 step 1 until m do
      A[ii, j] := A[ii, j] − A[i, j] × Amax;
      y[ii] := y[ii] − y[i] × Amax;
skip: end ii
  end i;
  ick := r + 1; for j := 1 step 1 until m do
  begin k := 1;
repeat: if j = ic[k] then go to next;
  k := k + 1; if r ≧ k then go to repeat;
  ic[ick] := j; ick := ick + 1;
next: end k;
  for i := r + 1 step 1 until n do
  begin for k := 1 step 1 until r do
    y[i] := y[i] − y[k] × A[i, ic[k]];
    for j := r + 1 step 1 until m do
    begin B[i, j] := A[i, ic[j]];
      for k := 1 step 1 until r do
      B[i, j] := B[i, j] − A[i, ic[k]] × A[k, ic[j]]
    end j
  end i;
  SURFIT (B, y[r+1:n], w[r+1:n], n − r, m − r, x[r+1:m],
    e[r+1:n], rms);
comment The procedure SURFIT is called to solve the reduced
  set of n − r simultaneous linear equations in m − r unknowns,
  Bx₂ = y₂′, which have no constraints;
for j := r + 1 step 1 until m do x[ic[j]] := x[j];
for j := 1 step 1 until r do
begin x[ic[j]] := y[j];
  for i := r + 1 step 1 until m do
  x[ic[j]] := x[ic[j]] − A[j, ic[i]] × x[ic[i]]
end j
end CONLSQ
```

REMARK ON ALGORITHM 177
LEAST SQUARES SOLUTION WITH CONSTRAINTS

[Michael J. Synge, Comm. ACM, June 63]

MICHAEL J. SYNGE
The Boeing Co., Transport Division, Renton, Wash.

In row-reducing the constraint equations, *CONLSQ* does not use full pivoting nor does it detect redundancy or inconsistency of the constraints; it was felt that the constraints were likely to be few in number and well-conditioned. However, these omissions may be made good by replacing the statement

$$ick := ick + 1;$$

by

$$done: ick := ick + 1;$$

and substituting the lines below for the first seven lines of the first compound statement of *CONLSQ*. If inconsistency is found, the procedure exits to the nonlocal label *inconsistent*. A roundoff tolerance, *eps*, is used in checking consistency, and some numerical value (e.g. 10^{-6}) should be substituted for it.

```
begin integer i, j, k, ii, ick, mr; integer array ic[1 : m];
    array B[1 : n−r, 1 : m−r];
  real Amax, Atemp;
  for i := 1 step 1 until r do
  begin k := 1; mr := i; Amax := A[i, 1];
    for ii := i step 1 until m do
    begin for j := 1 step 1 until m do
      begin if abs(Amax ≧ abs(A[ii, j]) then go to nogo;
        mr := ii; k := j; Amax := A[ii, j];
nogo: end j
    end ii;
    if abs(Amax) ≧ eps then go to allswell; mr := i;
test: if abs(y[mr]) ≧ eps then go to inconsistent else mr := mr + 1;
    if r ≧ mr then go to test else r := i − 1;
    go to done;
allswell: for j := 1 step 1 until r do
    begin Atemp := A[mr, j]; A[mr, j] := A[i, j];
      A[i, j] := Atemp/Amax
    end j;
    Atemp := y[mr]; y[mr] := y[i]; y[i] := Atemp/Amax:
```

The Algorithm then continues with the line:

```
    for ii := 1 step 1 until r do
```

ALGORITHM 178
DIRECT SEARCH

ARTHUR F. KAUPE, JR.
Westinghouse Electric Corp., Pittsburgh, Penn.

```
procedure direct search (psi, X DELTA, rho, delta, S);
value K, DELTA, rho, delta; integer K; array psi;
  real DELTA, rho, delta; real procedure S;
comment This procedure may be used to locate the minimum
  of the function S of K variables. A discussion of the use of this
  procedure may be found in: Robert Hooke and T. A. Jeeves,
  'Direct Search' Solution of Numerical and Statistical Problems
  [J. ACM 8, 2 (1961), 212-229]. The notation is essentially that
  used in Appendix B of the cited paper. The exceptions being the
  spelling of the Greek letters and the introduction of notation to
  distinguish between the process of calculating a value of S and
  the value itself—thus S(phi) and Sphi. A modified version of this
  procedure acceptable to the BAC compiler for the Burroughs
  205 and 220 computers has been prepared and run successfully;
begin real SS, Spsi, Sphi, theta; array phi [1:K]; integer K, k;
procedure E; for k := 1 step 1 until K do
  begin phi [k] := phi [k] + DELTA; Sphi := S(phi);
  if Sphi < SS then SS := Sphi else
    begin phi [k] := phi [k] - 2 × DELTA; Sphi := S(phi):
    if Sphi < SS then SS := Sphi else phi [k] := phi [k] + DELTA
  end E;
Start: Spsi := S(psi);
1: SS := Spsi;
for k := 1 step 1 until K do phi [k] := psi [k]; E;
if SS < Spsi then begin
  2: for k := 1 step 1 until K do begin
    theta := psi [k];
    psi [k] := phi [k];
    phi [k] := 2 × phi [k] - theta end;
  Spsi := SS; SS := Sphi := S(phi); E;
  if SS < Spsi then go to 2 else go to 1 end;
3: if DELTA ≥ delta then begin DELTA := rho × DELTA;
  go to 1 end end
```

REMARK ON ALGORITHM 178 [E4]
DIRECT SEARCH [Arthur F. Kaupe, Jr., *Comm. ACM* 6 (June 1963), 313]

M. BELL AND M. C. PIKE (Recd. 15 Nov. 1965 and 22 Apr. 1966)
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Algorithm 178 has the following syntactical errors:

(1) The parameter list should read

```
(psi,K,DELTA,rho,delta,S).
```

(2) The declaration

```
integer K,k;
```

should read

```
integer k;
```

(3) An extra **end** bracket is required immediately before **end** *E*;.

The algorithm compiled and ran after these modifications had been made but for a number of problems took a prodigious amount of computing owing to a flaw in the algorithm caused by rounding error. This flaw is in **procedure** *E* and may be illustrated by the one-dimensional case. Let $S(x) = 1.5 - x\ (x \leq 1.5)$, $3x - 4.5\ (x > 1.5)$, and start at 0 with a step of 1. The first move puts *psi* [1] = 1, *phi* [1] = 2. The second move should then put *phi* [1] = 1 = *psi*[1] resulting in a jump to label 1. On many machines, however, *E* will put *phi* [1] = 1 + *e* (*e*>0 and very small) so that direct search begins to move away from 1 in very small steps. This is clearly not desirable and may be avoided by altering the line

```
if SS < Spsi then go to 2 else go to 1 end;
```

to

```
if SS ≥ Spsi then go to 1;
for k := 1 step 1 until K do
if abs (phi[k]-psi[k]) > 0.5 × DELTA then go to 2
end;
```

To accelerate the procedure, direct search should take advantage of its knowledge of the sign of its previous move in each of the *K* directions. Take, for example, the one-dimensional case with starting point zero and the minimum far out and negative; the pattern moves will arrive there quite efficiently but each first move of *E* on the way will be positive whereas the previous experience of the search should lead it to suspect the minimum to be in the opposite direction.

Finally, two changes which we have found very useful are (i) some escape clause in the procedure to enable an exit to be made if the procedure has not terminated after some given number of function evaluations *maxeval*, with a Boolean *converge* taking the value **true** in general but **false** if the procedure has terminated through exceeding this number of function evaluations; and (ii) taking *Spsi* into the parameter list where it is called by name so that on exit *Spsi* contains the minimum value of the function.

With these modifications the procedure now reads:

```
procedure direct search (psi,K,Spsi,DELTA,rho,delta,S,converge,
    maxeval);
  value K,DELTA,rho,delta,maxeval; integer K,maxeval;
    array psi;
  real DELTA,rho,delta,Spsi; real procedure S; Boolean
    converge;
comment This procedure locates the minimum of the function S of
  K variables. The method used is that of R. Hooke and T. A.
  Jeeves ["Direct search" solution of numerical and statistical
  problems, J. ACM. 8 (1961), 212-229] and the notation used is
  theirs except for the obvious changes required by ALGOL. On
  entry: psi[1:K] = starting point of the search, DELTA =
  initial step-length, rho = reduction factor for step-length,
  delta = minimum permitted step-length (i.e. procedure is termi-
  nated when step-length < delta), maxeval = maximum per-
  mitted number of function evaluations. On exit: psi[1:K] =
  minimum point found and Spsi = value of S at this point,
  converge = true if exit has been made from the procedure be-
  cause a minimum has been found (i.e., step-length < delta)
  otherwise converge = false (i.e. maximum number of function
  evaluations has been reached);
begin integer k,eval; array phi,s[1:K]; real Sphi,SS,theta;
  procedure E;
  for k := 1 step 1 until K do
  begin phi[k] := phi[k] + s[k]; Sphi := S(phi); eval := eval
    + 1;
```

```
    if Sphi < SS then SS := Sphi else
    begin s[k] := - s[k]; phi[k] := phi[k] + 2.0 × s[k];
      Sphi := S(phi); eval := eval + 1;
      if Sphi < SS then SS := Sphi else
      phi[k] := phi[k] - s[k]
    end
  end E;
Start: for k := 1 step 1 until K do s[k] := DELTA;
  Spsi := S(psi); eval := 1; converge := true;
1: SS := Spsi;
  for k := 1 step 1 until K do phi[k] := psi[k]; E;
  if SS < Spsi then
  begin
2: if eval ≥ maxeval then
    begin converge := false;
      go to EXIT
    end;
    for k := 1 step 1 until K do
    begin if phi[k] > psi[k] ≡ s[k] < 0 then s[k] := -s[k];
      theta := psi[k]; psi[k] := phi[k]; phi[k] := 2.0 × phi[k] -
        theta
    end;
    Spsi := SS; SS := Sphi := S(phi); eval := eval + 1; E;
    if SS ≥ Spsi then go to 1;
    for k := 1 step 1 until K do
      if abs(phi[k]-psi[k]) > 0.5 × abs(s[k]) then go to 2
  end;
3: if DELTA ≥ delta then
  begin DELTA := rho × DELTA;
    for k := 1 step 1 until K do s[k] := rho × s[k]; go to 1
  end;
EXIT:
end direct search
```

REMARK ON ALGORITHM 178 [E4]

DIRECT SEARCH [Arthur F. Kaupe, Jr., *Comm. ACM 6* (June 1963), 313]

[as revised by M. Bell and M. C. Pike, *Comm. ACM 9* (Sept. 1966), 684]

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KEY WORDS AND PHRASES: function minimization, search, direct search

CR CATEGORIES: 5.19

The procedure does not exit, as specified, after *maxeval* (the maximum number of) function evaluations.

The 3 statements *eval* := *eval* +1 should be interchanged with the immediately preceding statement and replaced by a call to the procedure *test eval* defined below. The statement labeled 2 should be deleted.

```
  procedure test eval;
    if eval < maxeval then eval := eval +1
    else begin converge := false;
    go to EXIT
  end test eval
```

REMARK ON ALGORITHM 178 [E4]

DIRECT SEARCH [Arthur F. Kaupe, Jr., *Comm. ACM 6* (June 1963), 313]; [as revised by M. Bell and M. C. Pike, *Comm ACM 9* (Sept. 1966), 684]

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KEY WORDS AND PHRASES: function minimization, search, direct search

CR CATEGORIES: 5.19

The procedure *DIRECT SEARCH*, as modified by M. Bell and M. C. Pike [1], does not always provide the determined minimum. In addition, the maximum number of function evaluations permitted is almost always exceeded whenever the step-length is greater than *delta* at the time the number of function evaluations is greater than or equal to *maxeval*. Finally, the label 3 is not used.

To insure that the determined minimum is always provided, the test on the number of evaluations should be moved to a point where the minimum has been properly provided.

In [2] DeVogelaere remarks correctly that the procedure does not exit as specified and gives changes which will indeed cause the procedure to terminate when the number of function evaluations exceeds the specified limit (and not some number of evaluations later). However it is felt that DeVogelaere's solution to this problem causes excessive testing. Therefore the test should be performed after an exploratory move as in [1] but it should also be performed when the step-length is reduced. This method of testing violates the letter of the specified use of *maxeval* but not the intent, which is to provide an escape from excessive calculation.

To obtain the determined minimum, to provide a means for reducing the number of function evaluations when step-length is greater than *delta*, and to eliminate the unused label:

(1) The lines

```
2:  if eval ≥ maxeval then
      begin converge := false
        go to EXIT
      end;
```

should be removed.

(2) The line (16th line from the end of the procedure given in [1])

```
for k := 1 step 1 until K do
```

should be changed to

```
2:  for k := 1 step 1 until K do
```

(3) The line

```
Spsi := SS; SS := Sphi := S(phi); eval := eval + 1; E;
```

should have the following code inserted after the statement *Spsi* := *SS*;

```
if eval ≥ maxeval then
  begin
3:  converge := false;
    go to EXIT
  end;
```

(4) The line

```
3:  if DELTA ≥ delta then
```

should be changed to

if *DELTA* ≥ *delta* **then**

(5) The line
begin *DELTA* := *rho* × *delta*;

should be changed to

begin if *eval* > *maxeval* **then go to** 3 **else**
DELTA := *rho* × *delta*;

REFERENCES:
1. BELL, M., AND PIKE, M. C. Remark on Algorithm 178. *Comm. ACM 9* (Sept. 1966), 684.
2. DEVOGELAERE, R. Remark on Algorithm 178. *Comm. ACM 11* (July 1968), 498.

REMARK ON ALGORITHM 178 [E4]
DIRECT SEARCH [Arthur F. Kaupe, Jr., *Comm. ACM 6* (June 1963), 313; as revised by M. Bell and M. C. Pike, *Comm. ACM 9* (Sept. 1966), 684]

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KEY WORDS AND PHRASES: function minimization, search, direct search
CR CATEGORIES: 5.19

Algorithm 178, as modified by Bell and Pike [1], has been used successfully by the author on a number of different problems and in a variety of languages (e.g. Burroughs Extended ALGOL on a B5500, SUBALGOL on an IBM 7090, and FORTRAN on the IBM/360 series machines). A modification which has been found to be useful involves tailoring the step size to be meaningful for a wide variation in the magnitudes of the variables.

As currently specified [1], each variable is incremented (or decremented) by *DELTA* as a minimum is sought. For a function such that the values of the variables differ by several orders of magnitude at the minimum, a universal step size causes some parameters to be essentially ignored during much of the searching process. For example, if a function of two variables has a minimum near (100.0, 0.1), a step size of 10.0 will be useful in minimizing with respect to the first parameter, but it will be meaningless with respect to the second parameter until it has been reduced to near 0.01. On the other hand, a step size of 0.01 would be useful on the second variable but on the first variable it would take an undesirably large number of steps to approach the minimum.

A modification to direct search which circumvents this scaling problem involves the use of a different step size for each variable. This is easily implemented since an array is already used to hold the signed step size for each variable. The change is accomplished by removing the statement labeled *Start* and replacing it by the following statement:

```
Start: for k := 1 step 1 until K do
       begin s(k) := DELTA × abs (psi(k));
         if s(k) = 0.0 then s(k) := DELTA;
       end;
```

This change sets the step size for each variable to *DELTA* times the magnitude of the starting value, or if the starting value is 0.0 the step size is set equal to *DELTA*. Thus *DELTA* is the fraction of the original value of each variable to be used as an initial step size. Subsequent reductions in step size are handled correctly without further modifications to the procedure.

As an example of the usefulness of the above modification, consider the function

$$f(X_1, X_2, X_3) = (X_1 - 0.01)^2 + (X_2 - 1.0)^2 + (X_3 - 100.0)^2$$

with a minimum at (0.01, 1.0, 100.0). The following table shows the results of using direct search on this function with and without the modified step size. The results were computed on an IBM 360/75 computer using single precision with *rho* = 0.1, *delta* = 0.001, *DELTA* = 0.2 for the modified step size (giving 20 percent of initial value for initial step size) and *DELTA* = [average magnitude of initial guesses for the variables] for the algorithm as published.

TABLE I. $f = (X_1 - 0.01)^2 + (X_2 - 1.0)^2 + (X_3 - 100.0)^2$

	DELTA	*Number of function evaluations*	*Minimum value of f*	*Final values of the variables*		
				X_1	X_2	X_3
For initial values of (0.0, 0.0, 200.0):						
Direct search	66.6667	153	0.841×10^{-7}	0.00999995	0.999995	100.000
Modified direct search	.2	112	0.597×10^{-7}	0.00999998	0.999990	100.000
For initial values of (0.05, 5.0, 500.0):						
Direct search	168.35	174	0.934×10^{-7}	0.0100263	0.998958	99.9999
Modified direct search	.2	75	0.559×10^{-6}	0.00999988	0.999998	99.9992

Note that the modified method will tend to yield the same relative accuracy for each parameter, whereas with a fixed step size direct search will tend to give the same absolute accuracy for all parameters. In most cases a relative accuracy is probably more desirable than an absolute accuracy.

REFERENCES
1. BELL, M., AND PIKE, M. C. Remark on algorithm 178. *Comm ACM 9* (Sept. 1966), 684.

ALGORITHM 179
INCOMPLETE BETA RATIO*

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* Based in part on work done at Carnegie Institute of Technology, Pittsburgh, Pennsylvania and supported by the Petroleum Research Fund of the American Chemical Society and by the National Science Foundation.

```
real procedure incompletebeta (x, p, q, epsilon);
value x, p, q; real x, p, q, epsilon;
begin real finsum, infsum, temp, temp 1, term, term 1, qrecur, index;
  Boolean alter;
comment This procedure evaluates the ratio Bx(p, q)/B1(p, q),
  where Bx(p, q) = ∫0^x t^(p-1)(1-t)^(q-1) dt, with 0 ≦ x ≦ 1 and p, q > 0,
  but not necessarily integers. It assumes the existence of a non-
  local label, alarm, to which control is transferred upon entry to
  the procedure with invalid arguments. Also assumed is a proce-
  dure to evaluate ∫0^∞ t^p e^-t dt which is called factorial(p), (cf. e.g.
  Algorithm 80, March, 1962);
if x > 1 ∨ x < 0 ∨ p ≦ 0 ∨ q ≦ 0 then go to alarm;
if x = 0 ∨ x = 1 then begin incompletebeta := x; go to End end;
comment This part interchanges arguments if necessary to ob-
  tain better convergence in the power series below;
if x ≦ 0.5 then alter := false else
  begin alter := true; temp := p; p := q; q := temp; x :=
    1 - x end;
comment This part recurs on the (effective) q until the power
  series below does not alternate;
finsum := 0; term := 1; temp := 1 - x; qrecur := index := q;
for index := index - 1 while index > 0 do
  begin qrecur := index;
    term := term × (qrecur+1)/(temp×(p+qrecur));
    finsum := finsum + term
  end;
comment This part sums a power series for non-integral effec-
  tive q and yields unity for integer q;
infsum := term := 1; index := 0;
comment In the following statement the convergence criterion
  might well be altered to term > epsilon, since infsum > 1 al-
  ways, thus saving one divide per cycle at the cost, perhaps, of a
  few more cycles;
for index := index + 1 while (term/infsum) > epsilon do
  begin term := term × x × (index-qrecur) × (p+index-1)/
    (index×(p+index)); infsum := infsum + term
  end;
comment This part evaluates most of the necessary factorial
  functions, minimizing the number of entries into the factorial
  procedure;
temp := temp 1 := factorial (qrecur-1);
term := term 1 := factorial (qrecur+p-1);
for index := qrecur step 1 until (q-0.5) do
  begin temp 1 := temp 1 × index;
    term 1 := term 1 × (index+p)
  end;
comment This part combines the partial results into the final
  one;
  temp := x ↑ p × (infsum×term/(p×temp)+finsum×term 1×
  (1-x) ↑ q/(q×temp 1))/factorial (p-1);
incompletebeta := if alter then 1-temp else temp;
end: end incompletebeta
```

REMARK ON ALGORITHM 179 [S 14]
INCOMPLETE BETA RATIO [Oliver G. Ludwig, *Comm. ACM 6* (June 1963), 314]

M. C. PIKE AND I. D. HILL (Recd. 8 Oct. 1965 and 12 Jan. 1966)
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Algorithm 179 has the following two typographical errors:

(1) the line

```
if x ⩽ 0.5 then alter := false else
```

should read

```
if x ⩽ 0.5 then alter := false else
```

(2) the line

```
end:end incompletebeta
```

should read

```
End:end incompletebeta
```

With these changes Algorithm 179 ran successfully on the ICT Atlas computer using Algorithm 221 [Walter Gautschi, *Comm. ACM 7* (Mar. 1964), 143], to evaluate the factorials required. A minor improvement might be to call *epsilon* by value.

As the algorithm stands, the permitted range of p and q is dictated by overflow problems associated with finding the values of factorials. For most machines this will mean that $p+q$ will have to be less than about 70. In the statistical applications of this algorithm which we describe below this restriction is very serious. However, these factorials appear essentially only in the form of ratios, and by making use of this fact the permitted range of p and q can be enormously extended. This is most simply accomplished by using the real procedure *loggamma* [Algorithm 291, M. C. Pike and I. D. Hill, *Comm. ACM 9* (Sept. 1966), 684] modifying Algorithm 179 as follows: replace the instructions

```
temp := temp1 := factorial(qrecur-1);
```

to

```
temp := x ↑ p × (infsum×term/(p×temp)+finsum×term1×
(1-x) ↑ q/(q×temp1))/factorial(p-1);
```

inclusive, by

```
temp := x ↑ p × (infsum×exp(loggamma(qrecur+p)-loggamma
(qrecur)-loggamma(p+1.0))+finsum×(1.0-x) ↑ q
×exp(loggamma(p+q)-loggamma(p)-loggamma(q+1.0)));.
```

This also means that the declarations of *temp*1 and *term*1 are not required. For even moderately large values of p or q this will also have the effect of speeding up the algorithm [see Remark on Algorithm 291, M. C. Pike and I. D. Hill, *Comm. ACM 9* (Sept. 1966), 685].

The following real procedures use this algorithm to evaluate three of the most frequently required statistical distribution functions.

real procedure *Ftail* (*k*, *f1*, *f2*, *epsilon*);
value *k*, *f1*, *f2*, *epsilon*; **real** *k*, *f1*, *f2*, *epsilon*;
comment *Ftail* evaluates the probability that a random variable following an *F* distribution, on *f1* and *f2* degrees of freedom, exceeds a positive constant *k*;
Ftail := *incompletebeta*(*f2*/(*f2*+*f1*×*k*), 0.5×*f2*, 0.5×*f1*, *epsilon*);

real procedure *Student*(*k*, *f*, *epsilon*);
value *k*, *f*, *epsilon*; **real** *k*, *f*, *epsilon*;
comment *Student* evaluates the probability that the absolute value of a random variable following a *t* distribution, on *f* degrees of freedom, exceeds a positive constant *k*;
Student := *incompletebeta*(*f*/(*f*+*k* ↑ 2), 0.5×*f*, 0.5, *epsilon*);
real procedure *Binomial*(*k*, *n*, *p*, *epsilon*);
value *k*, *n*, *p*, *epsilon*; **real** *k*, *n*, *p*, *epsilon*;
comment *Binomial* evaluates the probability that a random variable following a binomial distribution, with parameters *n* and *p*, takes a value greater than or equal to *k*;
Binomial := *incompletebeta*(*p*, *k*, *n*−*k*+1.0, *epsilon*);

Remark on Algorithm 179 [S14]

Incomplete Beta Ratio

[Oliver G. Ludwig, *Comm. ACM* 6 (June 1963), 314]

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Description

Algorithm 179 (modified to include the remark by M.C. Pike and I.D. Hill [1]) computes the Incomplete Beta Ratio using this equation

$$I_x(p,q) = \frac{INFSUM \cdot x^p \cdot \Gamma(PS+p)}{\Gamma(PS)\cdot\Gamma(p+1)} + \frac{x^p\cdot(1-x)^q\cdot\Gamma(p+q)\,FINSUM}{\Gamma(p)\cdot\Gamma(q+1)}$$

INFSUM and *FINSUM* represent two series summations defined as follows:

$$INFSUM = \sum_{i=0}^{\infty} \frac{(1-PS)_i\cdot p}{p+i}\,\frac{x^i}{i!}, \text{ where}$$

$$(1-PS)_i = 1 \qquad [i=0]$$

$$= (1-PS)\cdot(2-PS)\cdots(i-PS) = \frac{\Gamma(1+i-PS)}{\Gamma(1-PS)} \qquad [i>0]$$

$$\text{and } FINSUM = \sum_{i=1}^{[q]} \frac{q\cdot(q-1)\cdots(q-i+1)}{(p+q-1)(p+q-2)\cdots(p+q-i)}\,\frac{1}{(1-x)^i},$$

where $[q]$ is equal to the largest integer less than q. If $[q] = 0$, then $FINSUM = 0$. PS is defined as

$PS = 1$, if q is an integer; otherwise
$= q - [q]$.

By rearranging Algorithm 179 so that scaling can be introduced, the argument range of p and q can be extended and accuracy can be improved.

Since $I_x(p, q)$ is a probability and, therefore, bounded [0, 1], and *INFSUM* and *FINSUM* are series having only positive terms, we see that $I_x(p, q)$ is a collection of terms all of which are positive and bounded in the range [0, 1] if: (1) each term of *INFSUM* is multiplied by $(x^p \cdot \Gamma(PS + p))/(\Gamma(PS) \cdot \Gamma(p + 1))$; and (2) each term of *FINSUM* is multiplied by $(x^p\cdot(1-x)^q\cdot\Gamma(p+q))/(\Gamma(p)\cdot\Gamma(q+1))$.

Knowing this fact, we can apply a scaling procedure to the algorithm. *INFSUM* is a decreasing series. If the product of the first term of *INFSUM* and its multiplicative factor would underflow, then the sum of this series could be set to zero and all calculations involving underflow could be avoided. This is handled in the modification of the algorithm given below. However, since *INFSUM* is a decreasing series, underflows may occur later in the calculations. No attempt has been made to handle them here.

The second summation is more complicated. The series is decreasing if $q/((q + p - 1)(1 - x))$ is less than 1. If an individual term becomes less than 1.*E*-6 times the previous sum, calculation can be legitimately terminated since no additivity is apparent. If a term of the decreasing series is less than an arbitrarily small constant (*EPS2*), calculation is also terminated. This is done to prevent underflows in the later terms.

If the series is increasing, the first terms may underflow. In this case a power of ϵ_1 (machine precision − 1.*E*-78 on the IBM 360/370) may be factored from each term in *FINSUM* (times its multiplier). These terms cannot be added to the sum since they are less than machine precision; however, they are useful in retaining the accuracy of the initial terms, which are then used recursively. By the nature of the problem, we know that any term in *FINSUM*, times its multiplier, must be less than or equal to 1, but we have factored out powers of ϵ_1. Therefore, if a term of *FINSUM* becomes greater than 1, we know that rescaling, by multiplying the term by ϵ_1, is in order.

Testing on the IBM 360/195 has shown that, by rearranging the calculations of the original Algorithm 179, and thus including scaling, the input range of the algorithm can be greatly extended with a high degree of accuracy.

MDBETA requires a double precision function *DLGAMA* which computes the log of the gamma function. ACM Algorithm 291 may be used. *MDBETA* was tested against the SSP routine *BDTR* given in the manual *System/360 Scientific Subroutine Package (360A-CM-03X) Version III Programmer's Manual*, H20-0205. *MDBETA* ran 3.5 times faster than *BDTR* with greater accuracy. For example, in the case $x = .5$, $p = 2000$ and $q = 2000$, *MDBETA* gave the correct result, .5, while *BDTR* gave an answer of .497026. The IMSL subroutine, *MDBIN*, was used for an additional comparison when p and q are integers. *MDBIN* maintains IBM 370/360 single precision accuracy (approximately six significant digits). Over the tests performed the maximum difference occurred in the fifth significant digit when p and q were less than 200. Three to four significant digits of accuracy can be expected with p and q as large as 2000.

Acknowledgments. The above ideas are the application of ideas learned from the late Hirondo Kuki. Routine *MDBETA* originated from a code which resides in IMSL Library 1. We thank Wayne Fullerton, from the University of California, Los Alamos Scientific Laboratory, for refereeing the paper.

Algorithm

```
      SUBROUTINE MDBETA(X, P, Q, PROB, IER)
C FUNCTION              - INCOMPLETE BETA PROBABILITY
C                           DISTRIBUTION FUNCTION
C USAGE       - CALL MDBETA (X,P,Q,PROB,IER)
C PARAMETERS
C   X     - VALUE TO WHICH FUNCTION IS TO BE INTEGRATED. X
C             MUST BE IN THE RANGE (0,1) INCLUSIVE.
C   P     - INPUT (1ST) PARAMETER (MUST BE GREATER THAN 0)
C   Q     - INPUT (2ND) PARAMETER (MUST BE GREATER THAN 0)
C   PROB  - OUTPUT PROBABILITY THAT A RANDOM VARIABLE FROM A
C             BETA DISTRIBUTION HAVING PARAMETERS P AND Q
C             WILL BE LESS THAN OR EQUAL TO X.
C   IER   - ERROR PARAMETER.
C             IER = 0 INDICATES A NORMAL EXIT
C             IER = 1 INDICATES THAT X IS NOT IN THE RANGE
C               (0,1) INCLUSIVE.
C             IER = 2 INDICATES THAT P AND/OR Q IS LESS THAN
C               OR EQUAL TO 0.
      DOUBLE PRECISION PS, PX, Y, P1, DP, INFSUM, CNT, WH, XE,
     * DQ, C, EPS, EPS1, ALEPS, FINSUM, PQ, D4, EPS2, DLGAMA
C DOUBLE PRECISION FUNCTION DLGAMA
C MACHINE PRECISION
      DATA EPS/1.D-6/
C SMALLEST POSITIVE NUMBER REPRESENTABLE
      DATA EPS1/1.D-78/
```

```
C NATURAL LOG OF EPS1
      DATA ALEPS/-179.6016D0/
C ARBITRARILY SMALL NUMBER
      DATA EPS2/1.D-50/
C CHECK RANGES OF THE ARGUMENTS
      Y = X
      IF ((X.LE.1.0) .AND. (X.GE.0.0)) GO TO 10
      IER = 1
      GO TO 140
   10 IF ((P.GT.0.0) .AND. (Q.GT.0.0)) GO TO 20
      IER = 2
      GO TO 140
   20 IER = 0
      IF (X.GT.0.5) GO TO 30
      INT = 0
      GO TO 40
C SWITCH ARGUMENTS FOR MORE EFFICIENT USE OF THE POWER
C SERIES
   30 INT = 1
      TEMP = P
      P = Q
      Q = TEMP
      Y = 1.D0 - Y
   40 IF (X.NE.0. .AND. X.NE.1.) GO TO 60
C SPECIAL CASE - X IS 0. OR 1.
   50 PROB = 0.
      GO TO 130
   60 IB = Q
      TEMP = IB
      PS = Q - FLOAT(IB)
      IF (Q.EQ.TEMP) PS = 1.D0
      DP = P
      DQ = Q
      PX = DP*DLOG(Y)
      PQ = DLGAMA(DP+DQ)
      P1 = DLGAMA(DP)
      C = DLGAMA(DQ)
      D4 = DLOG(DP)
      IF (Y.GT.EPS) GO TO 70
C SPECIAL CASE - X IS CLOSE TO 0. OR 1.
      XB = PX + PQ - D4 - P1 - C
      IF (XB.LE.ALEPS) GO TO 50
      PROB = DEXP(XB)
      GO TO 130
C DLGAMA IS A FUNCTION WHICH CALCULATES THE DOUBLE
C PRECISION LOG GAMMA FUNCTION
   70 XB = PX + DLGAMA(PS+DP) - DLGAMA(PS) - D4 - P1
C SCALING
      IB = XB/ALEPS
      INFSUM = 0.D0
C FIRST TERM OF A DECREASING SERIES WILL UNDERFLOW
      IF (IB.NE.0) GO TO 90
      INFSUM = DEXP(XB)
      CNT = INFSUM*DP
C CNT WILL EQUAL DEXP(TEMP)*(1.D0-PS)I*P*Y**I/FACTORIAL(I)
      WH = 0.0D0
   80 WH = WH + 1.D0
      CNT = CNT*(WH-PS)*Y/WH
      XB = CNT/(DP+WH)
      INFSUM = INFSUM + XB
      IF (XB/EPS.GT.INFSUM) GO TO 80
C DLGAMA IS A FUNCTION WHICH CALCULATES THE DOUBLE
C PRECISION LOG GAMMA FUNCTION
   90 FINSUM = 0.D0
      IF (DQ.LE.1.D0) GO TO 120
      XB = PX + DQ*DLOG(1.D0-Y) + PQ - P1 - DLOG(D0) - C
C SCALING
      IB = XB/ALEPS
      IF (IB.LT.0) IB = 0
      C = 1.D0/(1.D0-Y)
      CNT = DEXP(XB-FLOAT(IB)*ALEPS)
      PS = DQ
      WH = DQ
      P1 = (PS*C)/(DP+WH-1.D0)
      XB = P1*CNT
      IF (XB.LE.EPS2 .AND. P1.LE.1.D0) GO TO 120
  100 WH = WH - 1.D0
      IF (WH.LE.0.0D0) GO TO 120
      IF (P1.LE.1.D0 .AND. CNT/EPS.LE.FINSUM) GO TO 120
      CNT = (PS*C*CNT)/(DP+WH)
      IF (CNT.LE.1.D0) GO TO 110
C RESCALE
      IB = IB - 1
      CNT = CNT*EPS1
  110 PS = WH
      IF (IB.EQ.0) FINSUM = FINSUM + CNT
      GO TO 100
  120 PROB = FINSUM + INFSUM
  130 IF (INT.EQ.0) GO TO 140
      PROB = 1.0 - PROB
      TEMP = P
      P = Q
      Q = TEMP
  140 RETURN
      END
```

ACM Transactions on Mathematical Software, Vol. 2, No. 2, June 1976, Pages 207–208.

REMARK ON ALGORITHM 179

Incomplete Beta Ratio [S14]
[O. G. Ludwig, *Comm. ACM 6*, 6(June 1963), 314]

Malcolm C. Pike and Jennie SooHoo [Recd 5 March 1975 and 11 September 1975]
School of Medicine, University of Southern California, 1840 North Soto Street, Los Angeles, CA 90032

N. E. Bosten and T. J. Aird, International Mathematical and Statistical Libraries, Inc., 7500 Bellaire Blvd., Houston, TX 77036.

This work was supported by the Virus Cancer Program, National Cancer Institute, Bethesda, Md., under Grant PO ICA 17054-01 and Contract N01-CP-53500.

Algorithm 179 (*MDBETA*) can be improved as shown.

1. Remove *EPS2* from the double precision statement.

2. Remove the data statement and comment:

```
C       ARBITRARILY SMALL NUMBER
        DATA EPS2/1.D-50/
```

3. Remove the three statements preceding statement number 100:

```
P1=(PS*C)/(DP+WH-1.D0)
XB=P1*CNT
IF(XB.LE.EPS2.AND.P1.LE.1.D0) GO TO 120
```

4. After statement number 100, replace the following statements:

```
IF(P1.LE.1.D0.AND. CNT/EPS.LE.FINSUM) GO TO 120
CNT=(PS*C*CNT)/(DP+WH)
```

with the following:

```
      PX=(PS*C)/(DP+WH)
      IF(PX.GT.1.0D0) GO TO 105
      IF(CNT/EPS.LE.FINSUM .OR. CNT.LE.EPS1/PX) GO TO 120
  105 CNT=CNT*PX
```

The above changes eliminate the occurrence of underflow in the computation of *FINSUM* and decrease the execution time of the algorithm with no apparent change in accuracy.

5. Remove the statements and comment:

```
      IF(Y.GT.EPS) GO TO 70
C     SPECIAL CASE - X IS CLOSE TO 0. OR 1.
      XB=PX+PQ-D4-P1-C
      IF(XB.LE.ALEPS) GO TO 50
      PROB=DEXP(XB)
      GO TO 130
```

6. Remove the statement number from:

```
   70 XB=PX+DLGAMMA(PS+DP)-DLGAMMA(PS) - D4-P1
```

ALGORITHM 180
ERROR FUNCTION—LARGE X

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

```
real procedure erfL(x); value x; real x;
comment This procedure evaluates the error function of real
  argument, erf(x) = (2/√π) ∫_0^x e^-u^2 du by the Laplace continued
  fraction for the complementary error function: erf(x) = 1 -
  (1/(1+v/(1+2v/(1+3v/(1+···)))))/(√πx e^x^2) where v = 1/
  (2x^2). Successive even convergents of the continued fraction are
  evaluated, using an algorithm suggested by Maehly, until the
  full accuracy of the arithmetic being used is attained.
  The continued fraction converges for all x > 0. For small x,
  however, convergence may be excessively slow, and overflow
  may occur. In this region, the Taylor series converges satis-
  factorily, and algorithms such as No. 123 are suitable.
  For x ≦ 0, the procedure calls the global procedure alarm.
  The body of this procedure has been checked on the LGP-30
  computer, using the Dartmouth Self Contained Algol Processor.
  The program was used to tabulate erf(x) from 0.9(.1)5.0. The
  maximum error was 2 × 10^-6, which is explainable by roundoff
  errors. The number of convergents calculated ranged from 36
  for x = 0.9 to 2 for x ≧ 3.3. Overflow occurred for x = 0.87;
begin integer m; real B min 2, B min 3, P, R, T, v, v2;
if x ≤ 0 then alarm;
v := x × x;
T := -0.56418958/x/exp(v);
comment The constant 0.56418958 ··· = π^-1/2, and should
  be given to the full accuracy required of the procedure;
v := 0.5/v;
P = v × T;
v2 := v × v;
T := T + 1;
m := 0;
R := B min 3 := B min 2 := 1;
for m := m + 1 while T ≠ R do
  begin R := T;
  B min 3 := v × (m-1) × B min 3 + B min 2
  T := B min 2;
  B min 2 := v × m × B min 2 + B min 3;
  T := R - P/B min 2/T;
  P := m × (m+1) × v2 × P
  end while;
  erfL := T
end
```

REMARKS ON:
ALGORITHM 123 [S15]
REAL ERROR FUNCTION, ERF(x)
[Martin Crawford and Robert Techo *Comm. ACM 5* (Sept. 1962), 483]

ALGORITHM 180 [S15]
ERROR FUNCTION—LARGE *X*
[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 314]

ALGORITHM 181 [S15]
COMPLEMENTARY ERROR FUNCTION—LARGE *X*
[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 315]

ALGORITHM 209 [S15]
GAUSS
[D. Ibbetson. *Comm. ACM 6* (Oct. 1963), 616]

ALGORITHM 226 [S15]
NORMAL DISTRIBUTION FUNCTION
[S. J. Cyvin. *Comm. ACM 7* (May 1964), 295]

ALGORITHM 272 [S15]
PROCEDURE FOR THE NORMAL DISTRIBUTION FUNCTIONS
[M. D. MacLaren. *Comm. ACM 8* (Dec. 1965), 789]

ALGORITHM 304 [S15]
NORMAL CURVE INTEGRAL
[I. D. Hill and S. A. Joyce. *Comm. ACM 10* (June 1967), 374]

I. D. HILL AND S. A. JOYCE (Recd. 21 Nov. 1966)
Medical Research Council,
Statistical Research Unit, 115 Gower Street, London W.C.1., England

These algorithms were tested on the ICT Atlas computer using the Atlas ALGOL compiler. The following amendments were made and results found:

ALGORITHM 123

(i) **value** *x*; was inserted.
(ii) *abs*(*T*) ⩽ $_{10}-10$ was changed to $Y - T = Y$
both these amendments being as suggested in [1].
(iii) The labels 1 and 2 were changed to *L*1 and *L*2, the **go to** statements being similarly amended.
(iv) The constant was lengthened to 1.12837916710.
(v) The extra statement $x := 0.707106781187 \times x$ was made the first statement of the algorithm, so as to derive the normal integral instead of the error function.

The results were accurate to 10 decimal places at all points tested except $x = 1.0$ where only 2 decimal accuracy was found, as noted in [2]. There seems to be no simple way of overcoming the difficulty [3], and any search for a method of doing so would hardly be worthwhile, as the algorithm is slower than Algorithm 304 without being any more accurate.

ALGORITHM 180

(i) $T := -0.56418958/x/exp(v)$ was changed to $T := -0.564189583548 \times exp(-v)/x$. This is faster and also has the advantage, when v is very large, of merely giving 0 as the answer instead of causing overflow.

(ii) The extra statement $x := 0.707106781187 \times x$ was made as in (v) of Algorithm 123.
(iii) **for** $m := m + 1$ was changed to **for** $m := m + 2$. $m+1$ is a misprint, and gives incorrect answers.

The greatest error observed was 2 in the 11th decimal place.

ALGORITHM 181
(i) Similar to (i) of Algorithm 180 (except for the minus sign).
(ii) Similar to (ii) of Algorithm 180.
(iii) m was declared as **real** instead of **integer**, as an alternative to the amendment suggested in [4].

The results were accurate to 9 significant figures for $x < 8$, but to only 8 significant figures for $x = 10$ and $x = 20$.

ALGORITHM 209
No modification was made. The results were accurate to 7 decimal places.

ALGORITHM 226
(i) $10 \uparrow m/(480 \times sqrt(2 \times 3.14159265))$ was changed to $10 \uparrow m \times 0.000831129750836$.
(ii) **for** $i := 1$ **step** 1 **until** $2 \times n$ **do** was changed to $m := 2 \times n$; **for** $i := 1$ **step** 1 **until** m **do**.
(iii) $-(i \times b/n) \uparrow 2/8$ was changed to $-(i \times b/n) \uparrow 2 \times 0.125$.
(iv) **if** $i = 2 \times n - 1$ was changed to **if** $i = m - 1$
(v) $b/(6 \times n \times sqrt(2 \times 3.14159265))$ was changed to $b/(15.0397696478 \times n)$.

Tests were made with $m = 7$ and $m = 11$ with the following results:

x	*Number of significant figures correct*		*Number of decimal places correct*	
	$m = 7$	$m = 11$	$m = 7$	$m = 11$
−0.5	7	11	7	11
−1.0	7	10	7	10
−1.5	7	10	8	10
−2.0	7	9	8	10
−2.5	6	9	8	11
−3.0	6	7	8	9
−4.0	5	7	10	11
−6.0	2	1	12	10
−8.0	0	0	11	9

Perhaps the comment with this algorithm should have referred to decimal places and not significant figures. To ask for 11 significant figures is stretching the machine's ability to the limit, and where 10 significant figures are correct, this may be regarded as acceptable.

ALGORITHM 272
The constant .99999999 was lengthened to .9999999999.

The accuracy was 8 decimal places at most of the points tested, but was only 5 decimal places at $x = 0.8$.

ALGORITHM 304
No modification was made. The errors in the 11th significant figure were:

abs(x)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
0.5	1	1
1.0	1	2
1.5	21[a](5)	2
2.0	25[a](0)	4
3.0	0	0
4.0	2	3
6.0	6	0
8.0	14	0
10.0	23	0
20.0	35	0

[a] Due to the subtraction error mentioned in the comment section of the algorithm. Changing the constant 2.32 to 1.28 resulted in the figures shown in brackets.

To test the claim that the algorithm works virtually to the accuracy of the machine, it was translated into double-length instructions of Mercury Autocode and run on the Atlas using the EXCHLF compiler (the constant being lengthened to 0.39894228040143267793994 6). The results were compared with hand calculations using Table II of [5]. The errors in the 22nd significant figure were:

abs(x)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
1.0	2	3
2.0	7	1
4.0	2	0
8.0	8	0

Timings. Timings of these algorithms were made in terms of the Atlas "Instruction Count," while evaluating the function 100 times. The figures are not directly applicable to any other computer, but the relative times are likely to be much the same on other machines.

INSTRUCTION COUNT FOR 100 EVALUATIONS

abs(x)	Algorithm number							
	123	180	181	209	226 $m = 7$	272	304[a]	304[b]
0.5	58			8	97	24	25	24
1.0	65[c]			8	176	24	29	29
1.5	164	128	127	9	273	25	35	35
2.0	194	78	90	8	387	24	39	39
2.5	252	54	68	10	515	24	131	44
3.0		42	51	9	628	25	97	50
4.0		27	39	9	900[d]	25	67	44
6.0		15	30	6	1400[d]	16	49	23
8.0		9	28	7	2100[d]	18	44	11
10.0		10	25	5	2700[d]	16	38	11
20.0		9	22	5	6500[d]	16	32	11
30.0		9	9	5	10900[d]	16	11	11

[a] Readings refer to $x > 0 \equiv upper$.
[b] Readings refer to $x > 0 \not\equiv upper$.
[c] Time to produce incorrect answer. A count of 120 would fit a smooth curve with surrounding values.
[d] 100 times Instruction Count for 1 evaluation.

Opinion. There are advantages in having two algorithms available for normal curve tail areas. One should be very fast and reasonably accurate, the other very accurate and reasonably fast. We conclude that Algorithm 209 is the best for the first requirement, and Algorithm 304 for the second.

Algorithms 180 and 181 are faster than Algorithm 304 and may be preferred for this reason, but the method used shows itself in Algorithm 181 to be not quite as accurate, and the introduction of this method solely for the circumstances in which Algorithm 180 is applicable hardly seems worth while.

Acknowledgment. Thanks are due to Miss I. Allen for her help with the double-length hand calculations.

REFERENCES:

1. THACHER, HENRY C. JR. Certification of Algorithm 123. *Comm. ACM 6* (June 1963), 316.

2. IBBETSON, D. Remark on Algorithm 123. *Comm. ACM 6* (Oct. 1963), 618.

3. BARTON, STEPHEN P., AND WAGNER, JOHN F. Remark on Algorithm 123. *Comm. ACM 7* (Mar. 1964), 145.

4. CLAUSEN, I., AND HANSSON, L. Certification of Algorithm 181. *Comm. ACM 7* (Dec. 1964), 702.

5. SHEPPARD, W. F. *The Probability Integral.* British Association Mathematical Tables VII, Cambridge U. Press, Cambridge, England, 1939.

ALGORITHM 181
COMPLEMENTARY ERROR FUNCTION—LARGE X

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

```
real procedure erfcL(x); value x; real x;
comment This procedure evaluates the complementary error
  function, erfc(x) = 1 - erf(x) = (2/√π) ∫_x^∞ exp(-u²)du by
  the Laplace continued fraction:
    erfc(x) = (1/(1+v/(1+2v/(1+3v/(1+···)))))/(√π x e^{x²})
  where v = 1/(2x²). Successive even convergents of the continued
  fraction are evaluated, using an algorithm suggested by Maehly,
  until the full accuracy of the arithmetic being used is attained.
    The continued fraction converges for all x > 0. For small x,
  however, convergence may be excessively slow, and overflow
  and round-off accumulation may occur. In this region, the
  Taylor series converges satisfactorily.
    For x ≦ 0, the procedure calls the global procedure alarm.
    The body of this procedure has been checked on the LGP-30
  Computer, using the Dartmouth Self Contained Algol Processor,
  for x = 1.2(0.1)5.0. Results were generally correct to 1 in the
  6th significant digit, although a few errors were as large as 6
  in that digit. The errors are believed to be due to round-off
  only. The number of convergents calculated ranged from 46
  for x = 1.2 to 10 for x = 5.0.
    Overflow occurred for x = 1.183;
begin integer m; real B min 2, B min 3, P, R, T, v, v2;
if x ≤ 0 then alarm;
v := x × x;
T := 0.56418958/x/exp(v);
comment The constant 0.56418958 ··· = π^{-1/2}, and should be
  given to the full accuracy required of the procedure;
v := 0.5/v;
v2 := v × v;
P := v × T;
m := R := 0;
B min 3 := B min 2 := 1;
for m := m + 2 while R ≠ T do
  begin R := T;
  B min 3 := v × (m-1) × B min 3 + B min 2;
  T := B min 2;
  B min 2 := v × m × B min 2 + B min 3;
  T := R - P/B min 2/T;
  P := m × (m+1) × v2 × P
  end while;
  erfc L := T
end
```

CERTIFICATION OF ALGORITHM 181 [S15] COMPLEMENTARY ERROR FUNCTION—LARGE X [Henry C. Thacher, Jr., *Comm. ACM 6* (June 1963), 315]

I. CLAUSEN AND L. HANSSON (Recd. 20 Aug. 1964)
DAEC, Risø, Denmark.

The procedure *erfcL* was tested in GIER-ALGOL with 29 significant bits and the number-range $abs(x) < 2 \uparrow 512$ (approx. $1.3_{10}154$). The statement $m := R := 0;$ was corrected to $m := 0;$ $R := 0;$ [Because m and R are of different type; cf. Sec. 4.2.4 of the ALGOL Report, *Comm. ACM 6* (Jan. 1963), 1–17.—Ed.] After this the tests were successful. The procedure was checked a.o. for $x = 1.19$ (-0.01) 0.72. The differences from table values increased from $_{10}-8$ at $x = 1.1$ to $7_{10}-8$ at $x = 0.75$. Overflow occurred at $x = 0.71$.

REMARKS ON:
ALGORITHM 123 [S15] REAL ERROR FUNCTION, ERF(x)

[Martin Crawford and Robert Techo *Comm. ACM 5* (Sept. 1962), 483]

ALGORITHM 180 [S15] ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 314]

ALGORITHM 181 [S15] COMPLEMENTARY ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 315]

ALGORITHM 209 [S15] GAUSS

[D. Ibbetson. *Comm. ACM 6* (Oct. 1963), 616]

ALGORITHM 226 [S15] NORMAL DISTRIBUTION FUNCTION

[S. J. Cyvin. *Comm. ACM 7* (May 1964), 295]

ALGORITHM 272 [S15] PROCEDURE FOR THE NORMAL DISTRIBUTION FUNCTIONS

[M. D. MacLaren. *Comm. ACM 8* (Dec. 1965), 789]

ALGORITHM 304 [S15] NORMAL CURVE INTEGRAL

[I. D. Hill and S. A. Joyce. *Comm. ACM 10* (June 1967), 374]

I. D. HILL AND S. A. JOYCE (Recd. 21 Nov. 1966)
Medical Research Council,
Statistical Research Unit, 115 Gower Street, London W.C.1., England

These algorithms were tested on the ICT Atlas computer using the Atlas ALGOL compiler. The following amendments were made and results found:

ALGORITHM 123

(i) **value** x; was inserted.

(ii) $abs(T) < {}_{10}-10$ was changed to $Y - T = Y$

both these amendments being as suggested in [1].

(iii) The labels 1 and 2 were changed to *L1* and *L2*, the **go to** statements being similarly amended.
(iv) The constant was lengthened to 1.12837916710.
(v) The extra statement $x := 0.707106781187 \times x$ was made the first statement of the algorithm, so as to derive the normal integral instead of the error function.

The results were accurate to 10 decimal places at all points tested except $x = 1.0$ where only 2 decimal accuracy was found, as noted in [2]. There seems to be no simple way of overcoming the difficulty [3], and any search for a method of doing so would hardly be worthwhile, as the algorithm is slower than Algorithm 304 without being any more accurate.

ALGORITHM 180
(i) $T := -0.56418958/x/exp(v)$ was changed to $T := -0.564189583548 \times exp(-v)/x$. This is faster and also has the advantage, when v is very large, of merely giving 0 as the answer instead of causing overflow.
(ii) The extra statement $x := 0.707106781187 \times x$ was made as in (v) of Algorithm 123.
(iii) **for** $m := m + 1$ was changed to **for** $m := m + 2$. $m+1$ is a misprint, and gives incorrect answers.

The greatest error observed was 2 in the 11th decimal place.

ALGORITHM 181
(i) Similar to (i) of Algorithm 180 (except for the minus sign).
(ii) Similar to (ii) of Algorithm 180.
(iii) m was declared as **real** instead of **integer**, as an alternative to the amendment suggested in [4].

The results were accurate to 9 significant figures for $x \leqslant 8$, but to only 8 significant figures for $x = 10$ and $x = 20$.

ALGORITHM 209
No modification was made. The results were accurate to 7 decimal places.

ALGORITHM 226
(i) $10 \uparrow m/(480 \times sqrt(2 \times 3.14159265))$ was changed to $10 \uparrow m \times 0.000831129750836$.
(ii) **for** $i := 1$ **step** 1 **until** $2 \times n$ **do** was changed to $m := 2 \times n$; **for** $i := 1$ **step** 1 **until** m **do**.
(iii) $-(i \times b/n) \uparrow 2/8$ was changed to $-(i \times b/n) \uparrow 2 \times 0.125$.
(iv) **if** $i = 2 \times n - 1$ was changed to **if** $i = m - 1$
(v) $b/(6 \times n \times sqrt(2 \times 3.14159265))$ was changed to $b/(15.0397696478 \times n)$.

Tests were made with $m = 7$ and $m = 11$ with the following results:

x	*Number of significant figures correct*		*Number of decimal places correct*	
	$m = 7$	$m = 11$	$m = 7$	$m = 11$
−0.5	7	11	7	11
−1.0	7	10	7	10
−1.5	7	10	8	10
−2.0	7	9	8	10
−2.5	6	9	8	11
−3.0	6	7	8	9
−4.0	5	7	10	11
−6.0	2	1	12	10
−8.0	0	0	11	9

Perhaps the comment with this algorithm should have referred to decimal places and not significant figures. To ask for 11 significant figures is stretching the machine's ability to the limit, and where 10 significant figures are correct, this may be regarded as acceptable.

ALGORITHM 272
The constant .99999999 was lengthened to .9999999999.

The accuracy was 8 decimal places at most of the points tested, but was only 5 decimal places at $x = 0.8$.

ALGORITHM 304
No modification was made. The errors in the 11th significant figure were:

abs(x)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
0.5	1	1
1.0	1	2
1.5	21[a](5)	2
2.0	25[a](0)	4
3.0	0	0
4.0	2	3
6.0	6	0
8.0	14	0
10.0	23	0
20.0	35	0

[a] Due to the subtraction error mentioned in the comment section of the algorithm. Changing the constant 2.32 to 1.28 resulted in the figures shown in brackets.

To test the claim that the algorithm works virtually to the accuracy of the machine, it was translated into double-length instructions of Mercury Autocode and run on the Atlas using the EXCHLF compiler (the constant being lengthened to 0.39894228040143267793946). The results were compared with hand calculations using Table II of [5]. The errors in the 22nd significant figure were:

abs(x)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
1.0	2	3
2.0	7	1
4.0	2	0
8.0	8	0

Timings. Timings of these algorithms were made in terms of the Atlas "Instruction Count," while evaluating the function 100 times. The figures are not directly applicable to any other computer, but the relative times are likely to be much the same on other machines.

INSTRUCTION COUNT FOR 100 EVALUATIONS

abs(x)	Algorithm number							
	123	180	181	209	226 $m = 7$	272	304[a]	304[b]
0.5	58			8	97	24	25	24
1.0	65[c]			8	176	24	29	29
1.5	164	128	127	9	273	25	35	35
2.0	194	78	90	8	387	24	39	39
2.5	252	54	68	10	515	24	131	44
3.0		42	51	9	628	25	97	50
4.0		27	39	9	900[d]	25	67	44
6.0		15	30	6	1400[d]	16	49	23
8.0		9	28	7	2100[d]	18	44	11
10.0		10	25	5	2700[d]	16	38	11
20.0		9	22	5	6500[d]	16	32	11
30.0		9	9	5	10900[d]	16	11	11

[a] Readings refer to $x > 0 \equiv$ *upper*.
[b] Readings refer to $x > 0 \not\equiv$ *upper*.
[c] Time to produce incorrect answer. A count of 120 would fit a smooth curve with surrounding values.
[d] 100 times Instruction Count for 1 evaluation.

Opinion. There are advantages in having two algorithms available for normal curve tail areas. One should be very fast and reasonably accurate, the other very accurate and reasonably fast. We conclude that Algorithm 209 is the best for the first requirement, and Algorithm 304 for the second.

Algorithms 180 and 181 are faster than Algorithm 304 and may be preferred for this reason, but the method used shows itself in Algorithm 181 to be not quite as accurate, and the introduction of this method solely for the circumstances in which Algorithm 180 is applicable hardly seems worth while.

Acknowledgment. Thanks are due to Miss I. Allen for her help with the double-length hand calculations.

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ALGORITHM 182
NONRECURSIVE ADAPTIVE INTEGRATION

W. M. McKeeman and Larry Tesler
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```
real procedure Simpson(F) limits : (a, b) tolerance : (eps);
real procedure F; real a, b, eps; value a, b, eps;
begin comment A nonrecursive translation of Algorithm 145.
  Note that the device used here can be used to simulate recursion
  for a wide class of algorithms;
  integer lvl;
  switch return := r1, r2, r3;
  real array dx, epsp, x2, x3, F2, F3, F4, Fmp, Fbp,
  est2, est3 [1:30], pval[1:30, 1:3];
  integer array rtrn [1:30];
  real absarea, est, Fa, Fm, Fb, da, sx, est1, sum, F1;
  comment the parameter setup for the initial call;
  lvl := absarea := est := 0; da := b - a;
  Fa := F(a); Fm := 4.0 × F((a+b)/2.0); Fb := F(b);
  recur:
    lvl := lvl + 1; dx[lvl] := da/3.0;
    sx := dx[lvl]/6.0; Fl := 4.0 × F(a+dx[lvl]/2.0);
    x2[lvl] := a + dx[lvl]; F2[lvl] := F(x2[lvl]);
    x3[lvl] := x2[lvl] + dx[lvl]; F3[lvl] := F(x3[lvl]);
    epsp[lvl] := eps; F4[lvl] := 4.0 × F(x3[lvl]+dx[lvl]);
    Fmp[lvl] := Fm; est1 := (Fa+F1+F2[lvl]) × sx;
    Fbp[lvl] := Fb; est2[lvl] := (F2[lvl]+F3[lvl]+Fm) × sx;
                    est3[lvl] := (F3[lvl]+F4[lvl]+Fb) × sx;
    sum := est1 + est2[lvl] + est3[lvl];
    absarea := absarea - abs(est) + abs(est1) + abs(est2[lvl]) +
      abs (est3[lvl]);
    if (abs(est-sum) ≤ epsp[lvl] × absarea) ∨ (lvl≥30) then
    begin comment done on this level;
      up : lvl := lvl - 1;
      pval[lvl, rtrn[lvl]] := sum;
      go to return [rtrn[lvl]]
    end;
    rtrn[lvl] := 1; da := dx[lvl]; Fm := F1;
    Fb := F2[lvl]; eps := epsp[lvl]/1.7; est := est1;
    go to recur; r1:
    rtrn[lvl] := 2; da := dx[lvl]; Fa := F2[lvl];
    Fm := Fmp[lvl]; Fb := F3[lvl]; eps := epsp[lvl]/1.7;
    est := est2[lvl]; a := x2[lvl]; go to recur; r2:
    rtrn[lvl] := 3; da := dx[lvl]; Fa := F3[lvl];
    Fm := F4[lvl]; Fb := Fbp[lvl]; eps := epsp[lvl]/1.7;
    est := est3[lvl]; a := x3[lvl]; go to recur; r3:
    sum := pval[lvl, 1] + pval[lvl, 2] + pval[lvl, 3];
    if lvl > 1 then go to up;
  Simpson := sum
end Simpson
```

CERTIFICATION OF ALGORITHM 182
NONRECURSIVE ADAPTIVE INTEGRATION [W. M. McKeeman and Larry Tesler, *Comm. ACM 6* (June 1963), 315]

Harold S. Butler (Recd 8 Nov. 1963; rev. 6 Dec. 1963)
Stanford Linear Accelerator Center, Stanford, Calif.

A Balgol transliteration of *Simpson* has been prepared at Stanford by its authors and it has been used in a number of problems involving numerical integration. Its value was most strikingly displayed when it was utilized in a triple integral in which the final integration was over a strongly peaked function that spanned seven orders of magnitude. *Simpson* effectively minimized the number of evaluations and completed the integration five times faster than alternate schemes to subdivide the region of interest. The values of the integral agreed with independent calculations well within the required tolerance.

The following changes should be made to the published algorithm:

Line 13 should be changed to:

```
lvl := 0; absarea := est := 1.0; da := b-a;
```

Line 17 should read:

```
sx := dx[lvl]/6.0; F1 := 4.0 × F(a + dx[lvl]/2.0);
```

Line 20 should read:

```
epsp[lvl] := eps; F4[lvl] := 4.0 × F(x3[lvl] + dx[lvl]/2.0);
```

The condition of line 27 should be changed to:

```
if ((abs(est-sum) ≦ epsp[lvl] × absarea) ∧ (est ≠ 1.0)) ∨
  (lvl ≧ 30) then
```

ALGORITHM 183

REDUCTION OF A SYMMETRIC BANDMATRIX TO TRIPLE DIAGONAL FORM

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```
procedure bandred(a, n, m);
  value n, m; integer n, m; array a;
comment bandred reduces a real and symmetric matrix of band
  type (order n, a[i, k]=0 for |i−k|>m) by a sequence of orthog-
  onal similarity transformations to triple diagonal form. The
  procedure represents a generalization of the algorithm m21 by
  H. Rutishauser. Due to symmetry only the upper part of the
  band matrix must be given and these elements are denoted for
  convenience in the following way: a[i, 0] (i=1, 2, ···, n) repre-
  sents the diagonal element in the ith row, and a[i, k] (i=1, 2,
  ···, n−k and k=1, 2, ···, m) represents the generally nonzero
  element in the ith row and the kth position to the right of the
  diagonal. After completion of the reduction, the elements of the
  symmetric triple diagonal matrix are given by a[i, 0] (i=1, 2,
  ···, n) and a[i, 1] (i=1, 2, ···, n−1);
begin integer r, k, i, j, p, rr; real b, g, c, s, c2, s2, cs, u, v;
  for r := m step −1 until 2 do
  begin
    for k := 1 step 1 until n−r do
    begin
      for j := k step r until n−r do
      begin
        comment This compound statement describes the rota-
          tion involving the ith and (i+1)st rows and columns
          in order to reduce either a[j, r] or the off-band element
          g to zero, respectively. This rotation produces a new
          off-band element g (in general different from zero) pro-
          vided i + r < n;
        if j = k then
        begin if a[j, r] = 0 then go to endk;
          b := −a[j, r−1]/a[j, r]
        end
        else
        begin if g = 0 then go to endk;
          b := −a[j−1, r]/g
        end;
        s := 1/sqrt(1 + b×b); c := b × s;
        c2 := c × c; s2 := s × s; cs := c × s;
        i := j + r − 1;
cross elements:
        u := c2 × a[i, 0] − 2 × cs × a[i, 1] + s2 × a[i + 1, 0];
        v := s2 × a[i, 0] + 2 × cs × a[i, 1] + c2 × a[i+1, 0];
        a[i, 1] := cs × (a[i, 0] − a[i+1, 0]) + (c2−s2) ×a[i, 1];
        a[i, 0] := u; a[i+1, 0] := v;
column rotation:
        for p := j step 1 until i − 1 do
        begin
          u := c × a[p, i−p] − s × a[p, i−p+1];
          a[p, i−p+1] := s × a[p, i−p] + c × a[p, i−p+1];
          a[p, i−p] := u
        end p;
        if j ≠ k then
          a[j−1, r] := c × a[j−1, r] − s × g;
row rotation:
        rr := if r ≤ n − i then r else n − i;
        for p := 2 step 1 until rr do
        begin
          u := c × a[i, p] − s × a[i+1, p−1];
          a[i+1, p−1] := s × a[i, p] + c × a[i+1, p−1];
          a[i, p] := u
        end p;
        if i + r < n then
new g:  begin g := −s × a[i+1, r];
          a[i+1, r] := c × a[i+1, r]
        end
      end j;
endk: end k
  end r
end bandred
```

ALGORITHM 184

ERLANG PROBABILITY FOR CURVE FITTING

A. COLKER
U. S. Steel Applied Research Laboratory
Monroeville, Penn.

```
procedure ERLANG (X, XO, M, VARS, C, FACTORIAL, P);
value XO, M, VARS, C; integer C; real array X, P;
integer procedure FACTORIAL;
comment Computes the Erlang probability for the ith interval
  by ∫_0^{x_i} f(x)dx − ∫_0^{x_{i-1}} f(x)dx where f(x) = + [(Kμ)^K/(K−1)!]
  ·(x−x_0)^{K−1} e^{−Kμ(x−x_0)} where μ = 1/M, K = (M−X_0)²VARS is
  the upper boundary for the class intervals, X_0 is the lower
  boundary of the first class interval, M is the mean of the Er-
  lang, VARS is the variance corrected by Sheppard's correction,
  C is the number of class intervals and P_i is the calculated
  probability;
begin
  integer I, J, K, F; real array XE[0 : C];
    for I := 1 step 1 until C do
      XE[I] := X[I] − XO;
    XE[0] := 0;
    ME := M − XO;
    K := 0.5 + (ME↑2)/VARS;
    U := K/ME;
    SP := 0;
    for I := 1 step 1 until C do
    begin
        SUM1 := 0;
        SUM2 := 0;
        for J. := 0 step 1 until K − 1 do
        begin
          F := FACTORIAL (J);
          Z1 := U × XE[I−1];
      SUM1 := SUM1 + (Z1↑J)/F;
        Z2 := U × XE[I];
      SUM2 := SUM2 + (Z2↑J)/F;
    end J;
    P[I] := SUM1 × (EXP(−U×XE[I−1])) − SUM2
      × (EXP(−U×XE[I]));
    SP := SP + P[I];
  end I;
    P[C+1] := 1.0 − SP;
end Erlang
```

ALGORITHM 185
NORMAL PROBABILITY FOR CURVE FITTING
A. COLKER
U. S. Steel Applied Research Laboratory
Monroeville, Penn.

```
procedure NORMAL (X, M, VARS, C, HASTINGS, P);
value M, VARS, C; integer C; real array X, P;
real procedure HASTINGS;
comment Computes the normal probabilities for the ith interval
  by ∫_0^{x_i} f(x)dx − ∫_0^{x_{i-1}} f(x)dx where f(x) is Hastings' approxi-
  mation to the normal interval. Hastings' formula is

      φ(X_ni) = ½[1−(1+a1X_ni+a2X_ni^2+a3X_ni^3+a4X_ni^4+a5X_ni^5)^−8]

  where a1 = 0.09979268, a2 = 0.04432014, a3 = 0.00969920,
  a4 = −0.00009862, and a5 = 0.00058155. The X_ni are normalized
  boundary values of X_i where X_ni = (X_i−M)/√VARS, where
  M is the mean and VARS is the variance corrected by Sheppard's
  correction, C is the number of class intervals and P_i the calcu-
  lated probability;
begin
  integer I; real array XN[1 : C];
  for I := 1 step 1 until C do XN[I] := (X[I]−M)/SQRT(VARS);
  P[1] := 0.5 − HASTINGS (ABS(XN[1]));
  for I := 2 step 1 until C do
  begin
    if
  XN[I] < 0 then
  P[I] := HASTINGS (ABS(XN[I−1])) − HASTINGS
    (ABS(XN[I])); else
    begin
      if (XN[I]>0) ∧ (XN[I−1]<0)
      then P[I] := HASTINGS (XN[I]) + HASTINGS
        (ABS(XN[I−1])); else
      P[I] := HASTINGS (XN[I]) − HASTINGS (XN[I−1]);
    end;
  end I;
  P[C+1] := 0.5 − HASTINGS (XN[C]);
end NORMAL
```

ALGORITHM 186
COMPLEX ARITHMETIC

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```
procedure Complex arithmetic (a, b, R, r); value a, b; array
  a, b, R, r;
comment This procedure assigns the value a² + b² to R and the
  value (a+ib)/(a−ib) to r, where a, b, R and r are complex
  numbers. These two arithmetic expressions are of course fully
  arbitrary. They serve only to demonstrate the use of the pro-
  cedures P, Q, S, T, J and U. With them one can build up any
  arithmetic expression with complex variables, as easily as one
  can form them with real variables in ALGOL 60 (As one sees
  immediately these procedures can easily be extended for use in
  quaternion arithmetic or general vector and tensor calculus).
  We focus attention to the value call of the procedure-parameters,
  which is essential. Furthermore, we notice that the depth or
  height of the accumulator H is the number of right-handed
  brackets placed one after another not counting the brackets
which occur in parameter-delimeters. It is perhaps superfluous to
mention that this procedure was tested on the X1 computer of the
Mathematical Centre.;
begin integer i, k; array H[1:4,1:2];
  integer procedure P(i, j); value i, j; integer i, j;
  comment P forms the product of the ith and jth element of H;
  begin real a; k := k − 1; a := H[i, 1] × H[j, 1] − H[i, 2]
        × H[j, 2]; H[k, 2] := H[i, 1] × H[j, 2] + H[i, 2] ×
        H[j, 1]; H[k, 1] := a; P := k
  end;
  integer procedure Q(i, j); value i, j; integer i, j;
  comment Q forms the quotient of the ith and jth element of H;
  begin real a, b; k := k − 1; b := H[j, 1] ↑ 2 + H[j, 2] ↑ 2;
        a := (H[i, 1]×H[j, 1]+H[i, 2]×H[j, 2])/b;
        H[k, 2] := (H[i, 2]×H[j, 1]−H[i, 1]×H[j, 2])/b;
        H[k, 1] := a; Q := k
  end;
  integer procedure S(i, j); value i, j; integer i, j;
  comment S forms the sum of the ith and jth element of H;
  begin k := k − 1; H[k, 1] := H[i, 1] + H[j, 1];
        H[k, 2] := H[i, 2] + H[j, 2]; S := k
  end;
  integer procedure T(a); array a;
  comment T assigns to the k+1th element of H the complex
    variable a;
  begin k := k + 1; H[k, 1] := a[1]; H[k, 2] := a[2]; T := k
    end;
  integer procedure J(i, expi); integer i; real expi;
  comment J assigns to the (k+1)th element of H a complex
    variable which is decomposed in real and imaginary part;
  begin k := k + 1; i := 1; H[k, 1] := expi; i := 2;
        H[k, 2] := expi;
        J := k
  end;
  procedure U(i, R); value i; integer i; array R;
  comment U assigns to R the ith element of H;
  begin R[1] := H[i, 1]; R[2] := H[i, 2]; k := 0 end;
  k := 0; U(S(P(T(a))times:(T(a)))plus:(P(T(b))times:
    (T(b))), R);
  comment (a×a) + (b×b) =: R; U(Q(S(T(a)) plus:
    (P(J(i, i−1)) times: (T(b)))) divided by: (S(T(a))
    plus: (P(J(i, 1−i)) times: (T(b)))), r);
  comment (a+(i×b))/(a+(−i×b)) =: r;
end Complex Arithmetic;
```

The contents of this Algorithm are published in the Technical Note TN 27, Mathematical Centre, Nov. 1962.

ALGORITHM 187
DIFFERENCES AND DERIVATIVES

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Mathematical Centre, Amsterdam, Holland

```
begin real h; integer i, k; array A[1 : 50];
comment This program calculates, only to demonstrate the
  procedures DELTA and DER, the third derivative of the expo-
  nential function with a sixth order difference scheme. We do
  not propose to use these procedures in actual calculations, for
  as we observed with the X1 computer of the Math. Centre, they
  work, but very slowly as a consequence of the strong recursive-
  ness of the procedures. In actual programming one has to take
  the trouble to write out the well-known formula of Gregory, or
  for higher derivatives to multiply this formula a number of
  times by itself, then one has to collect the same function-values.
  All this trouble is taken over by the computer if one uses the
  procedures described below. My purpose, however, in publishing
  these procedures lies not in the numerical use but in a demon-
  stration of the flexibility of ALGOL 60, if one uses the recursive-
  ness property of procedures.;
 real procedure SUM(i, h, k, ti); value k; integer i, k, h;
   real ti;
 begin real s; s := 0; for i := h step 1 until k do s := s + ti;
       SUM := s
 end;
 real procedure DELTA (N, k, k0, fk); value N, k0; real fk;
 integer N, k, k0;
 comment N is the order of the forward difference which is
   calculated from a set of function-values with equidistant
   parameter-values;
 begin integer i;
       DELTA := if N = 1
       then SUM (k, k0, k0+1, (-1)↑(k+1-k0)×fk)
       else DELTA (1, i, k0, DELTA (N-1, k, i, fk))
 end;
 real procedure DER (OR, N, h, k, k0, fk); value OR, N, h, k0;
   real fk, h;
 integer OR, N, k, k0;
 comment OR is the order of the derivative, calculated from a
   given set of function-values f(k), with equidistant parameter-
   values, the error is of the order h ↑ (N+1-OR), where h is the
   steplength. k0 is the point where the derivative is calculated;
 begin integer i;
       DER := if OR = 1
       then SUM(i, 1, N, DELTA(i, k, k0, fk)
         ×(-1)↑(i+1)/i)/h
       else DER(1, N+1-OR, h, i, k0, DER(OR-1, N-1, h,
         k, i, fk))
 end;
 for i := 1 step 1 until 50 do A[i] := exp(i/50);
 for i := 1 step 1 until 25 do A[i] := DER(3, 6, .02, k, i, A[k])
end
```

The contents of this Algorithm are published in the Technical Note TN 27, Mathematical Centre, Nov. 1962.

ALGORITHM 188
SMOOTHING 1.
F. RODRIGUEZ-GIL
Central University, Caracas, Venezuela

```
procedure Smooth 13(n, x);
integer n;
real array x;
comment This procedure uses Gram's first-degree three-point
  formulas, as described in Hildebrand's "Introduction to Nu-
  merical Analysis," Ch. 7, to smooth a series of n equally spaced
  values. If the procedure is entered with less than three points,
  control is transferred to a nonlocal label error;
begin real array xp[1 : n]; integer i;
  if n < 3 then go to error;
  for i := 1 step 1 until n do xp[i] := x[i];
  x[1] := 0.83333333 × xp[1] + 0.33333333 × xp[2] − 0.16666667
    × xp[3];
  for i := 2 step 1 until n − 1 do x[i] := (xp[i−1]+xp[i]
    + xp[i+1]) × 0.33333333;
  x[n] := − 0.16666667 × xp[n−2] + 0.33333333 × xp[n−1]
    + 0.83333333 × xp[n]
end Smooth 13
```

ALGORITHM 189
SMOOTHING 2
F. RODRIGUEZ GIL
Central University, Caracas, Venezuela

```
procedure Smooth 35(n, x);
integer n;
real array x;
comment This procedure is similar to Smooth 13, except that
  Gram's third-degree five-point formulas are used, and that a
  minimum of five points is needed for a successful application;
begin real array xp[1 : n]; integer i;
  if n < 5 then go to error;
  for i := 1 step 1 until n do xp[i]:= x[i];
  x[1] := 0.98571429 × xp[1] + 0.05714286 × (xp[2]+xp[4])
    − 0.08571429 × xp[3] − 0.01428571 × xp[5];
  x[2] := 0.05714286 × (xp[1]+xp[5]) + 0.77142857 × xp[2]
    + 0.34285714 × xp[3] − 0.22857143 × xp[4];
  for i := 3 step 1 until n − 2 do x[i] := − 0.08571429 × (xp[i−2]
    +xp[i+2]) + 0.34285714 × (xp[i−1]+xp[i+1]) + 0.48571429
    × xp[i];
  x[n−1] := 0.05714286 × (xp[n−4]+xp[n]) − 0.22857143
    × xp[n−3] + 0.34285714 × xp[n−2] + 0.77142857 × xp[n−1];
  x[n] := − 0.01428571 × xp[n−4] + 0.05714286 × (xp[n−3]
    +xp[n−1]) − 0.08571429 × xp[n−2] + 0.98571429 × xp[n]
end Smooth 35
```

ALGORITHM 190
COMPLEX POWER
A. P. RELPH
The English Electric Co. Ltd., Whetstone, England

```
procedure Complex power (a, b, c, d, n, x, y); value a, b, c, d, n;
  real a, b, c, d, x, y; integer n;
comment This procedure calculates (x+iy) = (a+ib) ↑ (c+id)
  where i is the root of −1. In the complex plane, with a cut along
  the real axis from 0 to −∞, p is the sum of the principal value
  of the argument of (a+ib) and 2nπ (n is positive, negative or
  zero depending on the solution required). arctan is assumed to
  be in the range −π/2 to π/2. The case n = 0, d = 0 is given by
  Algorithm 106;
begin real p, r, v, w;
      if a = 0 then begin if b = 0 then begin x := y := 0;
                                        go to L end
                                      else p := 1.57079633 ×
                                        (sign(b)+4×n)
                    end
                else begin p := 6.28318532 × n + arctan(b/a);
                           if a < 0 then begin if b ≧ 0 then
                                                 p := p + 3.14159265
                                               else
                                                 p := p − 3.14159265
                                               end
                           end;
      r := .5 × ln(a↑2+b↑2); v := c × p + d × r;
      w := exp(c×r−d×p);
      x := w × cos(v); y := w × sin(v);
L: end
```

ALGORITHM 191
HYPERGEOMETRIC

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The English Electric Co. Ltd., Whetstone, England

```
procedure Hypergeometric (a1, a2, b1, b2, c1, c2, z1, z2) Results:
  (s1, s2); value a1, a2, b1, b2. c1, c2, z1, z2; real a1, a2, b1, b2,
  c1, c2, z1, z2, s1, s2;
begin comment calculates the hypergeometric function
        1F2(a, b, c, z) with complex parameters (a=a1+ia2,
        etc);
      real d, y1, y2; integer n;
      procedure comp mult (a1, a2, b1, b2, c1, c2); value a1,
        a2, b1, b2; real a1, a2, b1, b2, c1, c2;
        begin comment calculates the product of the two
                complex numbers (a1+ia2) and (b1+ib2)
                where i is the root of -1;
              c1 := a1 × b1 - a2 × b2; c2 := a2 × b1 +
                a1 × b2
        end;
      s1 := y1 := 1; s2 := y2 := 0;
      for n := 1 step 1 until 100 do
      begin d := n × ((c1+n-1)↑2+c2↑2);
            comp mult (a1+n-1, a2, y1/d, y2/d, y1, y2);
            comp mult (y1, y2, b1+n-1, b2, y1, y2);
            comp mult (y1, y2, c1+n-1, -c2, y1, y2);
            comp mult (y1, y2, z1, z2, y1, y2);
            if s1 = s1 + y1 ∧ s2 = s2 + y2 then go to L;
            s1 := s1 + y1; s2 := s2 + y2
      end;
L:  end
```

CERTIFICATION OF ALGORITHMS 191 AND 192 HYPERGEOMETRIC AND CONFLUENT HYPERGEOMETRIC [A. P. Relph, *Comm. ACM 6* (July 1963), 388]

HENRY C. THACHER, JR.* (Recd 2 Dec. 1963)
Argonne National Laboratory, Argonne, Ill

* Work supported by the U.S. Atomic Energy Commission.

The bodies of these two procedures were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. No syntactical errors were found, and the programs gave results agreeing within roundoff (7D) with tabulated values for the following special cases: ${}_2F_1(0.5, 0.5; 1; k^2) = (2/\pi)K(k)$; ${}_2F_1(0.5, -0.5; 1; k^2) = (2/\pi)E(k)$ where K and E are complete elliptic integrals of the first and second kinds; ${}_1F_1(.5; 1; iy) = J_0(x)$, and with ${}_1F_1(-1; 0.1; x)$; ${}_1F_1(-0.5; 0.1; x)$, and ${}_1F_1(-0.5; 0.5; x)$.

It should be observed that the function calculated by 191 is ${}_2F_1(a, b; c; z)$, not ${}_1F_2(a, b; c; z)$ as stated in the comment. These programs evaluate the functions by direct summation of the hypergeometric series. They are, therefore, relatively general, but inefficient. Precautions must also be taken against attempting to compute outside the range of effective convergence of the series.

Certification and Remark on Algorithm 191 [S22] Hypergeometric [A.P. Relph, *Comm. ACM 6* (July 1963), 388]

Henk Koppelaar (Recd. 14 Sept. 1973) Physical Laboratory, Division: Atom Physics, Utrecht State University, Utrecht, The Netherlands

The following changes were made in the algorithm:
(a) The subroutine for complex multiplication was erased.
(b) In accordance with (a) and with the standard notation ${}_2F_1$, the heading and end of the procedure were changed to read

```
real procedure hyp2geom1 (a, b, c, z);
end hyp2geom1.
```

(c) Erasing the subroutine for complex multiplication caused us to modify the algorithm further as follows.

```
  real procedure hyp2geom1 (a, b, c, z);
    value a, b c, z; real a, b, c, z;
  begin
    real s,y; integer i;
    s := y := 1;
    for i := 0 step 1 until 100 do
    begin
      y := y × ((a+i)/(c+i)) × (b+i) × z/(i+1);
      if s = s + y then go to exit; s := s + y
    end;
exit:
    hyp2geom1 := s
  end hyp2geom1
```

The inefficiency of the original algorithm for real arguments, as mentioned by Henry C. Thacher Jr. in his certification of it, is largely reduced by these modifications, because they make a considerable reduction in the computational costs.

With these modifications the algorithm was translated for the CDC-6500 using the Control Data Algol 3 compiler and ran only partially satisfactorily, as reported below.

The following two tests (a) and (b) were performed, using identities 1 and 2 and Algorithm 160 [1] for the combinatorial $\binom{m}{n}$. The identities are:

1. $(1/B(a\,b))\,(z^a/a)\,{}_2F_1(a, 1-b; a+1; z) = I_z(a, b)$,
2. $a \times B(a, b) = \binom{a+b-1}{a}^{-1}$, where

$$B(a, b) = \int_0^1 t^{a-1}(1-t)^{b-1}dt$$

is the complete beta function and

$$I_z(a, b) = (1/B(a, b)) \int_0^z t^{a-1}(1-t)^{b-1}dt$$

is the incomplete beta function, $a \geq 1, b \geq 1$, and a, b integer.

Test (a). Computing $\binom{a+b-1}{a} \times$ *hyp2geom1* $(a, 1-b, a+1, z) \times z \uparrow a$, gave correct results to 7D., according [2], for the following values of a, b and z.

$b = 7$,	$a = 7(1)9$	and z 0.61(0.01)0.97;
$b = 17$,	$a = 17$	and $z = 0.13$
$b = 17$,	$a = 17, 18$	and $z = 0.14$
$b = 17$,	$a = 17(1)19$	and $z = 0.15$
$b = 17$,	$a = 17(1)34$	and $z = 0.50$

The total computation time for this test using combinatorial and *hyp2geom1* was less than 10 sec on the Control Data 6500 computer.

Test (b). The same test as test (a) was performed for the following values of a, b, and z.

$b = 17$, $a = 17(1)34$ and $z = 0.51(0.01)0.60$.

The algorithm gave correct results to $5D$, according [2].

For the values

$b = 17$, $a = 17(1)34$ and $z = 0.61(0.01)0.89$, the results became worse with increasing z. This error is due to slower convergence of the series

$$ {}_2F_1\ (a, b; c; z) = \sum_{n=0}^{\infty} (a)_n (b)_n / (c)_n\ z^n/n! $$

with increasing z and increasing b.

Pochhammer's symbol means

$$ (a)_n = \Gamma(a+n)/\Gamma(a). $$

More precisely we see

$$ (1/B(a, b))(z^a/a)\ {}_2F_1\ (a, 1-b; a+1; z) = $$

$$ \sum_{n=0}^{\infty} \binom{a+b-1}{a} ((a)_n\ (1-b)_n/(a+1)_n)\ z^{n+a}/n! $$

From this expression it is clear that the rate of convergence of the expansion by and large is dominated by the values of b and z. This explains why in test (a) for $b = 7$ the results remained accurate to 7D for increasing z, and also it explains why in test (b) for $b = 17$ the results became worse for increasing z.

References

1. Wolfson, M.L., and Wright, H.V. Combinatorial of M things taken N at a time. *Comm. ACM 6*, 4 (Apr. 1963), 161.
2. Pearson, K. (Ed.). *Tables of the Incomplete Beta Function.* Cambridge U. Press, Cambridge, England, 1948.

ALGORITHM 192
CONFLUENT HYPERGEOMETRIC

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```
procedure Confluent hypergeometric (a1, a2, c1, c2, z1, z2)
  Result : (s1, s2); value a1, a2, c1, c2, z1, z2;
  real a1, a2, c1, c2, z1, z2, s1, s2;
begin comment calculates the confluent hypergeometric function
        1F1(a, c, z) with complex parameters
        (a=a1+ia2, etc);
      real d, y1, y2; integer n;
      procedure comp mult (a1, a2, b1, b2, c1, c2);
        value a1, a2, b1, b2; real a1, a2, b1, b2, c1, c2;
        begin comment calculates the product of the two
                complex numbers (a1+ia2) and (b1+ib2)
                where i is the root of -1;
              c1 := a1 × b1 - a2 × b2;
              c2 := a2 × b1 + a1 × b2
        end;
      s1 := y1 := 1; s2 := y2 := 0;
      for n := step 1 until 100 do
      begin d := n × ((c1+n-1)↑2+c2↑2);
            comp mult (a1+n-1, a2, y1/d, y2/d, y1, y2);
            comp mult (y1, y2, c1+n-1, -c2, y1, y2);
            comp mult (y1, y2, z1, z2, y1, y2);
          if s1 = s1 + y1 ∧ s2 = s2 + y2 then go to L;
          s1 := s1 + y1; s2 := s2 + y2
      end;
L: end
```

CERTIFICATION OF ALGORITHMS 191 AND 192 HYPERGEOMETRIC AND CONFLUENT HYPERGEOMETRIC [A. P. Relph, *Comm. ACM 6* (July 1963), 388]

HENRY C. THACHER, JR.* (Recd 2 Dec. 1963)
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

The bodies of these two procedures were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. No syntactical errors were found, and the programs gave results agreeing within roundoff (7D) with tabulated values for the following special cases: ${}_2F_1(0.5, 0.5; 1; k^2) = (2/\pi)K(k)$; ${}_2F_1(0.5, -0.5; 1; k^2) = (2/\pi)E(k)$ where K and E are complete elliptic integrals of the first and second kinds; ${}_1F_1(.5; 1; iy) = J_0(x)$, and with ${}_1F_1(-1; 0.1; x)$; ${}_1F_1(-0.5; 0.1; x)$, and ${}_1F_1(-0.5; 0.5; x)$.

It should be observed that the function calculated by 191 is ${}_2F_1(a, b; c; z)$, not ${}_1F_2(a, b; c; z)$ as stated in the comment. These programs evaluate the functions by direct summation of the hypergeometric series. They are, therefore, relatively general, but inefficient. Precautions must also be taken against attempting to compute outside the range of effective convergence of the series.

ALGORITHM 193
REVERSION OF SERIES

HENRY E. FETTIS
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```
procedure SERIESRVRT (A, B, N);
value A, N; array A, B; integer N;
comment This procedure gives the coefficients B[i] for the series
  x = y + ΣB[i] × y ↑ i (i=2, 3, ··· , n) when the coefficients
  A[i] of the series y = x + ΣA[i] × x ↑ i are given. The procedure
  uses successive approximations after writing y_{L+1} = x − ΣB[i] ×
  y_L ↑ i (i=2, 3, ··· , L+2 and L=0, 1, ··· , N−2) starting with
  y_0 = x;
begin integer i, j, k, m;
  array Q, R [0 : N];
  real s;
  A[1] := B[0] := 0;
  B[1] := 1;
  for k := 1 step 1 until N − 1 do
  begin B[k+1] := 0;
    for i := 0 step 1 until k + 1 do
    R[i] := 0;
    for j := k + 1 step − 1 until 1 do
    begin Q[0] := R[0] − A[j];
      for i := 1 step 1 until k + 1 do
      Q[i] := R[i];
      for i := 0 step 1 until k + 1 do
      begin s := 0;
        for m := 0 step 1 until i do
        s := s + B[m] × Q[i−m];
        R[i] := s
      end for i;
    end for j;
    for i := 2 step 1 until k + 1 do B[i] := R[i]
  end for k;
end SERIESRVRT
```

CERTIFICATION OF ALGORITHM 193
REVERSION OF SERIES [Henry E. Fettis, *Comm. ACM 5*, 1962]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

The body of Algorithm 193 was tested on the LGP-30 using the ALGOL 60 translator developed by the Dartmouth College Computer Center. No syntactical errors were found. The program successfully found the first four coefficients for the series for $ln(1+y)$ from the first four coefficients of the series for $y = e^x - 1$.

ALGORITHM 194
ZERSOL
CARLOS DOMINGO
Universidad Central, Caracas, Venezuela

```
procedure ZERSOL (h, YI, m, epsi, F, f, Z); real h, epsi, f;
  array YI, Z; integer m; procedure F;
comment ZERSOL finds the simple zeros of the solution Y1(Y0)
  of the set of m first order differential equations  Yj = Fj(Y0,
  Y1, ···, Ym).  h is the step of integration, epsi the error with
  which the zeros are to be determined (assuming no error in the
  process of integration). F(YS, j, v) is a procedure which calcu-
  lates the functions Fj, taking the arguments from the array
  YS and leaving the results in v. The search for zeros stops
  when Y0 > f. The zeros are stored as elements of the array Z.
  MR is a 4 × 4 matrix with the coefficients of a Runge-Kutta
  method. For example MR may be row-wise  0.5, 1, 0.5, 0, 1 − a,
  1 − a, 1 − a, 0.5, 1 + a, 1 + a, 1 + a, 0, ⅛, ⅛, 0.5, 0.5, where
  a = sqrt(2);
begin real v, r, d; integer j, s, n, k; array Q[1:m], YS[0:m],
  YAL [0:m], YT[1:m], MR[1:4,1:4]; switch S := NOZ, ZER;
  n := 1;
for d := h while YI[0] ≦ f do
  begin s := 1;
    R1: for j := 1 step 1 until m do
        begin Q[j] := 0.0; YS[j] := YI[j]; YT[j] := YI[j] end;
          YS[0] := YI[0];
    R2: for k := 1 step 1 until 4 do
        begin YS[0] := YS[0] + MR[k, 4] × d;
          for j := 1 step 1 until m do
         begin F(YS,j,v); v := v × d;
           r := MR[k,1] × v − MR[k,2]× Q[j];
           YT[j] := YT[j] + r;
           Q[j] := Q[j] + 3.0 × r − MR[k,3] × v
         end;
         for j := 1 step 1 until m do YS[j] := YT[j]
         end;
        go to S(s);
  NOZ: if sign(YI[1]) ≠ sign(YS[1]) then go to IT;
    TR: for j := 0 step 1 until m do YI[j] := YS[j]; go to R2;
    IT: s := 2;
        for j := 0 step 1 until m do YAL[j] := YS[j];
  ZER: d := d/2;
    if d ≦ epsi then go to STZ;
    if sign(YI[1]) = sign(YS[1]) then go to TR else go to R1;
  STZ: Z[n] := YI[0] := YI[0] + d; n := n + 1;
       for j := 0 step 1 until m do YI[j] := YAL[j]
  end;
end
```

ALGORITHM 195
BANDSOLVE
DONALD H. THURNAU
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```
procedure BANDSOLVE (C,N,M,V); value N,M; integer
  N,M; real array C,V;
comment BANDSOLVE is effective in solving the matrix equa-
  tion AX = B when the matrix A is of large order and sparse
  such that a narrow band centered on the main diagonal includes
  all the non-zero elements. Parameter N is the order of A, and M
  is the width of the band, necessarily an odd number of elements.
  BANDSOLVE is very efficient because it operates only on the
  band portion of the matrix A, given in the N by M array C. The
  band elements of a given row of A appear in the same row of C
  but shifted such that element A[i,j] becomes C[i,j-i+(M+1)/2].
  All band elements whether zero or non-zero must be given. The
  values of undefined elements of C, such as C[1,1] or C[N,M], are
  irrelevant. The array V initially contains the vector B. After
  solution, the array V contains the answer vector X. The con-
  tents of array C are destroyed during solution which is done by
  Gauss elimination with row interchanges, followed by back sub-
  stitution;
begin integer JM,LR,I,PIV,R,J; real T;
  LR := (M+1) ÷ 2;
  for R := 1 step 1 until LR - 1 do
    for I := 1 step 1 until LR - R do
      begin for J := 2 step 1 until M do
        C[R,J-1] := C[R,J];
        C[R,M] := C[N+1-R,M+1-I] := 0
      end of row shifting and zero placement;
  for I := 1 step 1 until N - 1 do
    begin PIV := I;
      for R := I + 1 step 1 until LR do
        if abs(C[R,1])>abs(C[PIV,1]) then
          PIV := R;
      if PIV ≠ I then
        begin T := V[I];
          V[I] := V[PIV];
          V[PIV] := T;
          for J := 1 step 1 until M do
            begin T := C[I,J];
              C[I,J] := C[PIV,J];
              C[PIV,J] := T
            end J
        end of row interchange;
      V[I] := V[I]/C[I,1];
      for J := 2 step 1 until M do
        C[I,J] := C[I,J]/C[I,1];
      for R := I + 1 step 1 until LR do
        begin T := C[R,1]
          V[R] := V[R] - T × V[I];
          for J := 2 step 1 until M do
            C[R,J-1] := C[R,J] - T × C[I,J];
          C[R,M] := 0
        end R;
      if LR ≠ N then LR := LR + 1
    end of triangularization;
  V[N] := V[N]/C[N,1];
  JM := 2;
    for R := N - 1 step -1 until 1 do
      begin for J := 2 step 1 until JM do
        V[R] := V[R] - C[R, J] × V[R-1+J];
      if JM ≠ M then JM := JM + 1
      end of back solution
end BANDSOLVE
```

Remark on Algorithm 195 [F4]

BANDSOLVE [Donald H. Thurnau, *Comm. ACM 6* (Aug. 1963), 441]

Ernst Schuegraf [Recd. 1 Mar. 1971]
Department of Mathematics, St. Francis Xavier University, Antigonish, Nova Scotia, Canada

Algorithm 195 was transliterated into Fortran IV for the IBM 360/50. Various matrices with different values of N and M were used. The execution time was recorded and the accuracy of the results was checked.

Execution time [sec]

	$M = 11$	$M = 15$	$M = 21$	$M = 25$
$N = 50$	.2	.7	1.1	1.9
$N = 100$	.6	1.6	2.5	4.2

The execution time shows the expected proportionality to $((M - 1) \div 2)^2 \cdot N$. (Note the definition of M!) When checking the results, it was found that the algorithm failed for singular and near singular matrices. To protect against this, it is recommended to introduce a tolerance *eps* for a test on singularity and a label *fail*. This requires the following changes in the procedure declaration:

```
procedure BANDSOLVE (C,N,M,V,eps,fail);
```

It is necessary to insert the following statements in the blockhead of the procedure:

```
real eps; label fail;
```

After the statement *piv* := *r*; insert:

```
if abs (C[piv, 1]) < eps go to fail;
```

ALGORITHM 196
MULLER'S METHOD FOR FINDING ROOTS OF AN ARBITRARY FUNCTION

ROBERT D. RODMAN
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```
procedure MULLER (p1, p2, p3, mxm, nrts, ep1, ep2, sw1, sw2,
  sw3, swr, rrt, irt);
value p1, p2, p3, mxm, nrts, ep1, ep2, sw1, sw2, sw3, swr;
integer mxm, nrts; boolean sw1, sw2, sw3, swr;
real p1, p2, p3, ep1, ep2; array rrt, irt;
begin comment procedure MULLER finds real and complex
  roots of an arbitrary function. p1, p2, and p3 are starting values.
  Roots nearest these points are found first. mxm is the maximum
  number of iterations to be made in finding any one root. ep1 and
  ep2 are specified as tolerance parameters. If ABS((X[i+1]-X[i])/
  X[i+1]) < ep1 or if the function value and modified function value
  are both less than ep2, a root has been found. If sw1 is true,
  then each iterant of each root is printed. If sw2 is true, the
  value of each root found is printed. If sw3 is true, then, when
  applicable, the complex conjugate of each root found is admitted
  as a root. If swr is true, only real roots are found. rrt and irt
  contain the real, and imaginary parts of each root found. Procedure
  function is the function generator and procedure complex performs
  necessary complex operations;
boolean bool; integer c1, rtc, i, itc; real rx1, rx2, rx3, ix1,
  ix2, ix3, rroot, iroot, rdnr, idnr, t1, it1, frroot, firoot, rfx1, rfx2,
  rfx3, ifx1, ifx2, ifx3, rh, ih, rlam, ilam, rdel, idel, t2, it2, t3, it3, t4,
  it4, rg, ig, rden, iden, rfunc, ifunc;
switch j := m2, m3, m4, m7, m11;
procedure function (reale, imag, reval, ieval);
value reale, imag; real reale, imag, reval, ieval;
begin comment Coding for this procedure must be inserted at
  compile time. reale and imag are the real and imaginary parts
  of the dependent variable. reval and ieval, the real and imaginary
  parts of the function;
end function;
procedure complex (a, ia, b, ib, k, c, ic);
value a, ia, b, ib, k; integer k;
real a, ia, b, ib, c, ic;
begin real temp; switch j := mpy, dvd, sqt;
      go to j[k];
mpy:  c := a × b − ia × ib; ic := a × ib + ia × b; go to exit;
dvd:  if (ib=0) ∧ (b=0) then begin ic := 0; c := 1;
      go to exit end; temp := b ↑ 2 + ib ↑ 2;
      c := (a×b+ia×ib)/temp; ic := (ia×b−a×ib)/temp;
      go to exit;
sqt:  if (ia=0) ∧ (a<0) then
      begin c := 0; ic := sqrt (−a) end
      else if ia = 0 then
      begin c := sqrt(a); ic := 0 end
      else begin temp := sqrt (a↑2+ia↑2);
        c := sqrt ((temp + a)/2);
        ic := if (temp − a) < 0 then 0
          else sqrt ((temp − a)/2) end;
      if ((b+c)↑ 2 + (ib+ic)↑ 2) < ((b−c)↑ 2 + (ib−ic)↑ 2)
      then begin c := b − c; ic := ib − ic end
      else begin c := b + c; ic := ib + ic end;
exit: end of complex;
start: for i := 1 step 1 until nrts do rrt [i] := irt [i] := 0; rtc := 0;
m0:   ix1 := ix2 := ix3 := c1, := iroot := itc := 0;
      rroot := p1; bool := false;
m1:   c1; := c1 + 1; rdnr := 1; idnr := 0;
      for i := 1 step 1 until rtc do
        begin
          complex (rdnr, idnr, rroot-rrt [i], iroot-irt [i], 1, t1, it1);
            rdnr := t1; idnr := it1
        end;
      function (rroot, iroot, t1, it1);
      complex (t1, it1, rdnr, idnr, 2, frroot, firoot);
      go to j[c1];
m2:   rfx1 := frroot; ifx1 := firoot; rroot := p2;
      go to m1;
m3:   rfx2 := frroot; ifx2 := firoot; rroot := p3;
      go to m1;
m4:   rfx3 := frroot; ifx3 := firoot; rx1 := p1;
      rx2 := p2; rx3 := p3; rh := rx3 − rx2;
      ih := ix3 − ix2;
      complex (rh, ih, rx2− rx1, ix2− ix1, 2, rlam, ilam);
      rdel := rlam + 1; idel := ilam;
m9:   if (rfx1=rfx2) ∧ (rfx2=rfx3) ∧ (ifx1=ifx2) ∧ (ifx2=ifx3)
      then begin rlam := 1; ilam := 0; go to m8 end;
      complex (rfx1, ifx1, rlam, ilam, 1, t1, it1);
      complex (rfx2, ifx2, rdel, idel, 1, t2, it2);
      t1 := t1 − t2 + rfx3; it1 := it1 − it2 + ifx3;
      complex (rdel, idel, rlam, ilam, 1, t2, it2);
      complex (t1, it1 t2, it2, 1, t3, it3);
      complex (rfx3, ifx3, t3, it3, 1, t1, it1);
      t1 := −4 × t1; it1 := −4 × it1;
      complex (rfx3, ifx3, rlam+rdel, ilam+idel, 1, t2, it2);
      complex (rdel↑2−idel↑2, 2×rdel×idel, rfx2, ifx2, 1, t3, it3);
      complex (rlam↑2−ilam↑2, 2×rlam×ilam, rfx1, ifx1, 1,
        t4, it4);
      rg := t4 − t3 + t2; ig := it4 − it3 + it2;
      if swr ∧ ((rg↑2+t1)<0) then
        begin rden := rg; iden := ig := 0 end
      else complex (rg↑2−ig↑2+t1, 2×rg×ig+it1, rg, ig, 3,
        rden, iden);
      complex (−2×rfx3, −2×ifx3, rdel, idel, 1, t1, it1);
      complex (t1, it1, rden, iden, 2, rlam, ilam);
m8:   itc := itc + 1;
      rx1 := rx2; rx2 := rx3; rfx1 := rfx2; rfx2 := rfx3;
      ix1 := ix2; ix2 := ix3; ifx1 := ifx2; ifx2 := ifx3;
      complex (rlam, ilam, rh, ih, 1, t1, it1);
      rh := t1; ih := it1;
m6:   rdel := rlam + 1; idel := ilam; rx3 := rx2 + rh;
      ix3 := ix2 + ih; c1 := 3; rroot := rx3;
      iroot := ix3; go to m1;
m7:   rfx3 := frroot; ifx3 := firoot;
      function (rx3, ix3, rfunc, ifunc);
      complex (rfx3, ifx3, rfx2, ifx2, 2, t1, it1);
      if (t1↑2+it1↑2) > 100 then
        begin rlam := rlam/2; rh := rh/2; ilam := ilam/2;
          ih := ih/2; go to m6 end;
      if sw1 then . . .
comment option to output iterant and associated function
  values;
  t1 := rx3 − rx2; it1 := ix3 − ix2;
  complex (t1, it1, rx2, ix2, 2, t2, it2);
```

```
  if sqrt (t2↑2+it2↑2) ≦ ep1 then go to fin1;
  if (sqrt (rfx3↑2+ifx3↑2)≦ep2) ∧
  (sqrt (rfunc↑2+ifunc↑2)≦ep2) then go to fin 2;
  go to if itc ≧ mxm then fin3 else m9;
fin1: if sw2 then . . .
comment option to output root; go to m12;
fin2: if sw2 then . . .
comment option to output root; go to m12;
fin3: if sw2 then . . .
comment no convergence, option to output last iterant;
  bool := true;
m12: rtc := rtc + 1; rrt[rtc] := rx3; irt[rtc] := ix3;
     if rtc ≧ nrts then go to exit;
     if (ABS(ix3)>ep1) ∧ sw3 ∧ ¬ bool then
       begin ix3 := −ix3; function (rx3, ix3, rfunc, ifunc);
         rroot := rx3; iroot := ix3; c1 := 4;
         go to m1;
m11: if sw2 then . . .
comment the complex conjugate of the last root found is acceptable. Option to output this root;
   rtc := rtc + 1; rrt[rtc] := rx3; irt[rtc] := ix3
    end else go to m0;
  if rtc < nrts then go to m0;
exit: end of procedure MULLER
```

CERTIFICATION OF ALGORITHM 196 [C5] MULLER'S METHOD FOR FINDING ROOTS OF AN ARBITRARY FUNCTION [Robert D. Rodman, *Comm. ACM 6* (Aug. 1963), 442]

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KEY WORDS AND PHRASES: equation roots, function zeros
CR CATEGORY: 5.15

The Algorithm. Algorithm 196 has been compiled in FORTRAN IV on the CDC-3600 and the IBM-7090 both in single and in double precision. The single precision versions used the system-supplied complex arithmetic subroutines; the double precision versions used subroutines agreeing as closely as possible with those described in the IBJOB Manual [4]. Thus, the algorithm tested differs from the published algorithm only in the complex square root subroutine.

There are five remarks to be made about Algorithm 196.

(1) As the Algorithm stands, if one of the values $P1$, $P2$, or $P3$ is a root of the equation and if more than one root is to be found, then the procedure will fail with a 0/0 form in the computation of

$$F_r(z) = f(z)/\prod_{i=1}^{rtc}(z-z_i).$$

Our decision was to terminate the procedure with a message to the user. The referee has suggested an alternative:

```
m1: rdnr := 1; idnr := 0;
    for i := 1 step 1 until rtc do
  begin
  if rroot = rrt [i] ∧ iroot < irt [i] then
  begin
    if c1 = 0 then P1 := rroot := 2 × rroot + ep1 else
    if c1 = 1 then P2 := rroot := 2 × rroot + ep1 else
    if c1 = 2 then P3 := rroot := 2 × rroot + ep1 else
    begin comment we have converged to a zero found previously, we accept it without any test;
      go to fin1;
    end;
      go to m1
      end;
      complex (rdnr, idnr, rroot − rrt [i], iroot − irt [i], 1, t1,
      it1); rdnr := t1; idnr := it1
  end;
  c1 := c1 + 1;
  function (rroot, iroot, t1, it1);
```

(2) The logical variable *bool* should be called by name in the procedure statement and should be an array of the same dimension as *rrt* and *irt*. Otherwise, unless *sw2* is *true*, the user will not know which of the "roots" satisfies the convergence criteria and which was returned by default.

(3) The statement *fin2* is unnecessary, since it is identical to *fin1*.

(4) Frank [1] states, "This procedure (Muller's method) works readily for functions having simple roots. On the other hand, if a function possesses multiple roots, ξ, then $F_r(z)$ is indeterminate when z approaches a ξ which may already have been found. However, even in this case the process has never failed. In fact, roots of multiplicity six or more have been found successfully. This is primarily due to the fact that multiple roots are found to much less accuracy than simple roots and behave, in effect, like clustered roots." In a private communication, Frank explained that the subroutine described in [1] included steps which perturbed roots already found, forcing them to behave like clustered roots. Frank's remark is not true for Algorithm 196, as a simple test with $(z-2)^2$, requesting two roots, will demonstrate.

(5) The complex square root in procedure *complex* contains at least two errors, not the least of which is that it fails to take account of the location of the complex number whose root is being computed. The referee has pointed out a second error: "The 5th line after the line labelled *sqt* should be

$$c := sqrt((temp+a)/2) \times sign(ia).$$

The construct **if** $(temp-a) < 0$ **then** 0 is unnecessary as the Boolean expression cannot be true. Moreover, even with corrections the complex square root included is unsatisfactory because, when ia is small, either $temp - a$ or $temp + a$ will be a difference of two nearly equal numbers and loss of significance will occur."

It is suggested that the four lines beginning four lines below the label *sqt* be replaced by

```
  else begin temp := sqrt((abs(a)+sqrt(a↑2+ia↑2))/2);
    ic := .5 × ia/temp;
    if a ≥ 0 then c := temp
    else begin c := abs(ic);
      ic := sign(ia) × temp
    end;
  end;
  if ((b+c)↑2+(ib+ic)↑2) < ···
```

Under some systems, the case $ia = -0$ might cause problems. With the possible exception of the case $ia = -0$, this coding will choose the square root whose real part is positive.

Modifications to the Algorithm. Both the single and double precision versions have been altered as suggested by Traub [3, p. 212]:

$$z_{i+1} = z_i - \frac{2f_i}{\rho_i}, \quad f_i = f(z_i)$$

$$\rho_i = \omega_i \pm \{\omega_i^2 - 4f_i f[z_i, z_{i-1}, z_{i-2}\}^{\frac{1}{2}}$$

$$\omega_i = f[z_i, z_{i-1}] + (z_i - z_{i-1})f[z_i, z_{i-1}, z_{i-2}]$$

$$f[z_i, z_{i-1}, z_{i-2}] = \frac{f[z_i, z_{i-1}] - f[z_{i-1}, z_{i-2}]}{z_i - z_{i-2}}$$

$$f[z_i, z_{i-1}] = \frac{f_i - f_{i-1}}{z_i - z_{i-1}}$$

Both Algorithm 196 and Traub's iteration function choose the sign of the square root to maximize the modulus of the denominator.

Although the two iteration functions are equivalent, Traub's requires fewer operations (8 additions, 5 multiplications and 3 divisions compared to Muller's 10 additions, 15 multiplications and 2 divisions), less storage and less computing time.

The behavior of the coded version of Traub's method differed little from that of Algorithm 196. Given the same starting values, both methods converged in the same number of iterations, even though the first iterates were sometimes different. Example 1 compares Muller and Traub in single precision with double precision. The difference between the first iterates in single precision is the result of roundoff due to the fact that the initial function values, $f(P1), f(P2)$, and $f(P3)$, are very close together. In double precision the two methods agreed to 17 significant figures (the CDC-3600 carries approximately 24 decimal digits in double precision).

Comparison of double versus single precision results on the same machine and double versus double (single versus single) on two different machines have been made. In every case differences can be satisfactorily explained by (1) different BCD-binary conversion on different machines, (2) different word lengths, or (3) differences in library subroutines on the various machines.

Example 1. $f(z) = z^{20} - 1$

$P1 = .1875$ $f(P1) = -.99999999999999715799543$ $ep1 = .5_{10} - 6$
$P2 = .375$ $f(P2) = -.99999999697569621957785$ $ep2 = .5_{10} - 6$
$P3 = .5$ $f(P3) = -.99999904632468349375000$ $nrts = 2$

	CDC-3600 Iteration		z		$f(z)$	
1	s.p.	Alg.196	8.959044683	−001	−8.890227259	−001
		Traub	8.959064917	−001	−8.890177130	−001
	d.p.		8.9590562323582572	−001	−8.8901986473910256	−001
2	s.p.	Alg.196	1.009184101	+000	2.006266970	−001
		Traub	1.009182792	+000	2.005955638	−001
	d.p.		1.0091833539604292	+000	2.0060892685123016	−001
3	s.p.	Alg.196	9.915438059	−001	−1.562027260	−001
		Traub	9.915451528	−001	−1.561798028	−001
	d.p.		9.9154457471920591	−001	−1.5618964171373523	−001
4	s.p.	Alg.196	9.996899988	−001	−6.181798671	−003
		Traub	9.996900961	−001	−6.179863674	−003
	d.p.		9.9969005435603457	−001	−6.1806941810976143	−003
5	s.p.	Alg.196	9.999986299	−001	−2.740146010	−005
		Traub	9.999986307	−001	−2.738516196	−005
	d.p.		9.9999863036901786	−001	−2.7392263226776617	−005
6	s.p.	Alg.196	1.000000000	+000	3.492459655	−009
		Traub	1.000000000	+000	3.492459655	−009
	d.p.		1.0000000001972048	+000	3.9440963812509629	−009

Example 2. Acoustic Waveguide Function

$f(z) = P\frac{\sin(2\pi S)}{S} + \rho\cos(2\pi S)$, $\rho = 2.50$

$P = \sqrt{(k^2 - z^2)}$, $Re(P) < 0$; $S = \sqrt{[(z/\epsilon)^2 - k^2]}$, $Re(s) < 0$;
$k = 0.0$, $\epsilon = 0.288$; $P1 = 0.0$, $P2 = 0.02$, $P3 = 0.04$

Iteration	$z = x + iy$		$f(z) = u + iv$	
	x	y	u	v
1	0.67672247−01	0.44008261−02	0.24001462−00	0.49014466−01
2	0.71677143−01	0.51274250−02	0.23259824−01	0.98558515−02
3	0.72102452−01	0.53056952−02	0.20655826−03	0.19331276−07
4	0.72106262−01	0.53092607−02	0.39539112−07	0.40978193−07

Example 3. The 20 Roots of Unity

Starting values at approximately 19, 27, and 35 degrees. Conjugates accepted as roots. $ep1 = ep2 = .5_{10} - 7$. Roots are at $e^{ir\pi/10}$, $r = 0, \cdots, 19$.

Root	r	Number of iterations
0	3	5
1	17	*
2	4	15
3	16	*
4	7	22
5	13	*
6	9	14
7	11	*
8	5	14
9	15	*
10	1	10
11	19	*
12	2	7
13	18	*
14	6	10
15	14	*
16	0	5
17	8	8
18	12	*
19	10	2

* Asterisk in column 3 indicates conjugate taken; i.e., $z_1 = \bar{z}_0$, $z_3 = \bar{z}_2$, etc.

Miscellaneous Comments. Both versions of Muller's method (Algorithm 196 and Traub's iteration function) have the advantage over other one-point-with-memory methods in that it is possible to locate complex zeros using real starting values. There is, of course, the possibility of spending unnecessary time doing complex arithmetic. As a general purpose library routine, unless one is looking for complex zeros, there are other iterative functions that require less space and have the same order; there are also others requiring less space and enjoying higher order, although they usually involve computing derivatives. For our purposes, the Traub version of Muller's method has proved quite satisfactory.

Example 2 is included to indicate the behavior of the Algorithm using a non-algebraic function. With this function both Algorithm 196 and the Traub modification agreed exactly except for a difference in the last digit in the first iterate.

Example 3 is included to show the order in which the 20 roots of unity are found and the number of iterations required to attain the specified accuracy. Values were checked against the NBS *Tables of Sines and Cosines to 15 Decimal Places*. All but two roots were correct to 9 significant figures; the remaining two were correct to 8.

Acknowledgment. The support of this work by the Atomic Energy Commission, Contract AT(29-2)-1163, is gratefully acknowledged.

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ALGORITHM 197
MATRIX DIVISION

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```
procedure Pos Div (b, c, m, n, solve);
value m, n, solve; array b, c; integer m, n; Boolean solve;
comment The matrix c, with m rows and n columns, is divided
  by the positive definite matrix b, of order m, by the square root
  method (see Fadeeva, V. N., Computational Methods of Linear
  Algebra, Chap 2, §10). The upper triangle of b is replaced by
  an upper triangular matrix N such that N^tN = b. The other
  elements of b are undisturbed. The matrix c is replaced by b^-1c.
  The Boolean solve is used as a switch. If its value is true, then
  it is assumed that an earlier entry to Pos Div has left the matrix
  N in place, and a further division of c by b takes place;
begin integer i, j, k;
  real procedure dot (a, b, p, q);
  value q; real a, b; integer p, q;
  comment This is innerproduct, modified to define a function
    designator;
  begin real s; s := 0;
  for p := 1 step 1 until q do s := s + a × b;
  dot := s end dot;
  Start of program: if solve then go to back substitution;
  for i := step 1 until m do
  begin b [i, i] := sqrt (b[i, i] - dot (b[j, i]↑2, 1, j, i - 1));
    for j := i + 1 step 1 until m do
    b[i,j] := (b[i,j] - dot (b[k,i], b[k,j], k, i-1))/b[i,i]
  end formation of upper triangular matrix;
back substituton: for i := 1 step 1 until n do
  begin for j := 1 step 1 until m do
    c[i,j] := (c[i,j] - dot (b[k,j], c[i,k], k, j-1))/b[j,j];
      for j := m step -1 until 1 do
    c[i,j] := (c[i,j] - dot (b[j,m+1-k], c[i,m+1-k], k, m-j))/
      b[j,j]
  end of double back substitution
end of Pos Div
```

CERTIFICATION OF ALGORITHM 197
MATRIX DIVISION [M. Wells, *Comm. ACM 6* (Aug. 1963), 443]

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The procedure was tested on a Ferranti Pegasus, using the ALGOL compiler developed by the de Havilland Aircraft Company at Hatfield. The line after the one labelled 'start of program' should read

for i := 1 **step** 1 **until** m **do**

(the first 1 was omitted).

The statement labelled *back substituton* is incorrect, and should read

```
back substitution: for j := 1 step 1 until n do
begin  for i := 1 step 1 until m do
  c[i,j] := (c[i,j] - dot (b[k,i], c[k,j], k,i-1))/b[i, i];
    for i := m step -1 until 1 do
  c[i,j] := (c[i,j] - dot (b[i,m+1-k],  c[m+1-k,j], k,m-i))/b[i,i]
end of double back substitution
```

With these changes the program was operated successfully on a number of small test problems. The procedure is only applicable to symmetric positive definite matrices, and no systematic attempt has yet been made to assess the accuracy of the results.

The word 'symmetric' should be inserted before 'positive definite' in the comment.

It is interesting to note that the original, incorrect version of the procedure will divide one symmetric matrix by another, and so can be used for matrix inversion.

ALGORITHM 198
ADAPTIVE INTEGRATION AND MULTIPLE INTEGRATION

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```
begin comment This program illustrates the declaration and
  call of a procedure used to numerically approximate definite
  integrals and multiple integrals. The integrand is an expression
  substituted for the first formal parameter and must be a func-
  tion of the simple variable replacing the second formal pa-
  rameter. Multiple integration is accomplished by substituting
  a complete call of Integral for the first formal parameter. Note
  that in this case that the limits of integration on the inside calls
  may be functions of the variable of integration on the outer
  call. The parameter rule selects a Newton-Cotes formula which
  matches a polynomial of degree = rule to the function in the
  interval of integration. (See Hamming, Numerical Methods for
  Scientists and Engineers, Sec. 12.2). In any case, the procedure
  integral adapts its step size to the function in seeking to mini-
  mize the number of function evaluations. The program has been
  tested and run on a variety of functions using the ALGOL com-
  piler on the Burroughs B-5000.;
real procedure Integral (F) a function of the real variables: (x)
  between limits: (a,b) polynomial degree: (rule) tolerance: (eps);
value a, b, rule, eps; integer rule;
real F, x, a, b, eps;
begin comment set up the parameters for the recursion before
  calling the procedure NC;
switch nct := R1, R2, R3, R4, R5, R6, R7;
real array cf, fn [1:rule+1];
integer k; real da, ab;
real procedure NC(F,x,a,da,fn,k,cf,rule,eps,es,ab,1v1);
value a, da, rule, eps, es, 1v1; real array cf;
integer k, rule, 1v1; real F, x, a, da, fn, eps, es, ab;
begin comment NC is the adaptive heart of Integral;
  real array fc[1:rule+1,1:rule+1], est, xx[1:rule+1];
  integer i, j; real dx, int, ep;
  real procedure SUM(term, index, upperlimit);
  real term; integer index, upperlimit;
  begin real t; t := 0;
    for index := 1 step 1 until upperlimit do
      t := t + term;
    SUM := t
  end of SUM;
  comment begin the integration by evaluating F on the mesh
    points;
  for k := 1 step 1 until rule + 1 do fc[k,k] := fn;
  dx := da/(rule×(rule+1));
  x := a;
  for i := 1 step 1 until rule + 1 do
    for j := 1 step 1 until rule do
    begin
      if j = 1 then xx[i] := x;
      if i ≠ j then fc[i,j] := cf[j] × F;
      x := x + dx;
    end having done all necessary function evaluations;
  for i := 1 step 1 until rule do
    fc[i, rule+1] := fc[i+1,1];
  ep := eps/sqrt(rule+1);
  comment eps/(rule + 1) is the value to give an absolute
    error bound of eps in the final answer. It proves too strict in
    practice;
  dx := dx × rule;
  comment compute the integrals of the subintervals;
  for i := 1 step 1 until rule + 1 do
    est[i] := SUM(fc[i,j],j,rule+1)×dx;
  ab := ab − abs(es) + SUM(abs(est[i]),i,rule+1);
  comment ab is the area under abs(F). It is used in computing
    the relative error upon which to terminate;
  int := SUM(est[i],i,rule+1);
  if 1v1 ≧ 100/(rule+1) then go to error;
  NC := if abs(es−int) ≦ eps × ab ∧ es ≠ 1.0 then int
    else SUM(NC(F,x,xx[i],dx,fc[i,j],j,cf,rule,ep,est[i], ab,1v1+1),
      i,rule+1);
  go to return;
  error; NC := int;
    comment abs(es − int) is the approximate error caused by
      terminating the recursion. In most cases, termination at
      this level will not adversely affect the accuracy of the result;
  return:
end of NC;
comment now initialize the Newton-Cotes coefficients;
go to nct [rule];
R1: cf[1] := cf[2] := 1.0/2.0; go to compute;
R2: cf[1] := cf[3] := 1.0/6.0; cf[2] := 4.0/6.0;
comment R1 is trapezoidal rule, R2 is Simpson's rule;
go to compute;
R3: cf[1] := cf[4] := 1.0/8.0;
    cf[2] := cf[3] := 3.0/8.0; go to compute;
R4: cf[1] := cf[5] := 7.0/90.0;
    cf[2] := cf[4] := 32.0/90.0;
    cf[3] := 12.0/90.0; go to compute;
R5: cf[1] := cf[6] := 19.0/288.0;
    cf[2] := cf[5] := 75.0/288.0;
    cf[3] := cf[4] := 50.0/288.0; go to compute;
R6: cf[1] := cf[7] := 41.0/840.0;
    cf[2] := cf[6] := 216.0/840.0;
    cf[3] := cf[5] := 27.0/840.0;
    cf[4] := 272.0/840.0; go to compute;
R7: cf[1] := cf[8] := 75.1/1728.0;
    cf[2] := cf[7] := 357.7/1728.0;
    cf[3] = cf[6] := 134.3/1728.0;
    cf[4] := cf[5] := 298.9/1728.0;
compute: da := b − a;
for k := 0 step 1 until rule do
begin
  x := a + k × da/rule;
  fn[k+1] := F × cf[k+1];
end;
ab := 1.0;
    Integral := NC(F,x,a,da,fn[k],k,cf,rule,eps,1.0,ab,0);
  end of Integral;
  comment Now evaluate the integral of 1.0/sqrt(abs(x+y))
    on the unit disk in the x,y-plane;
  real x, y, answer;
  answer := Integral(Integral(1.0/sqrt(abs(x+y)), x,
    −sqrt(1.0−y↑2), sqrt(1.0−y↑2), 7, 0.001),y,−1.0,1.0,3,0.001);
end of program;
```

ALGORITHM 199
CONVERSIONS BETWEEN CALENDAR DATE AND JULIAN DAY NUMBER

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```
procedure JDAY (d,m,y,j);
integer d,m,y,j;
comment JDAY converts a calendar date, Gregorian calendar,
  to the corresponding Julian day number j. From the given day
  d, month m, and year y, the Julian day number j is computed
  without using tables. The procedure is valid for any valid
  Gregorian calendar date. When transcribing JDAY for other
  compilers, be sure that integers of size 3 × 10⁶ can be handled;
begin integer c, ya;
  if m > 2 then m := m − 3
    else begin m := m + 9; y := y − 1 end;
  c :=y ÷ 100; ya := y −100 × c;
  j := (146097×c)÷4+(1461×ya)÷4+(153×m+2)÷5+d+1721119
end JDAY
```

```
procedure JDATE (j,d,m,y);
integer j,d,m,y;
comment JDATE converts a Julian day number j to the corre-
  sponding calendar date, Gregorian calendar. Since j is an integer
  for this procedure, it is correct astronomically for noon of the
  day. JDATE computes the day d, month m, and year y, without
  using tables. The procedure is valid for any valid Gregorian
  calendar date. When transcribing JDATE for other compilers,
  be sure that integers of size 3 × 10⁶ can be handled:
begin j := j − 1721119;
  y := (4×j−1) ÷ 146097; j := 4×j − 1 − 146097 × y;
    d := j÷ 4;
  j := (4×d+3) ÷ 1461; d := 4×d + 3 − 1461 × j;
    d := (d + 4) ÷ 4;
  m := (5×d−3) ÷ 153; d := 5×d − 3 − 153 × m;
    d :=(d+5) ÷ 5;
  y := 100 × y + j; if m < 10 then m := m + 3
    else begin m := m − 9; y := y + 1 end;
end JDATE
```

```
procedure KDAY (d,m,ya,k);
integer d,m,ya,k;
comment KDAY converts a calendar date, Gregorian calendar,
  to the corresponding serial day number k. From the given day
  d, month m, and the last two decimals of the year, ya, the serial
  day number k is computed without using tables. The procedure
  is valid from 1 March 1900 (k=1) to 31 December 1999
  (k = 36465). To obtain the Julian day number j (valid at noon)
  use j = k + 2415079;
begin if m > 2 then m := m − 3
    else begin m := m + 9; ya := ya − 1 end;
  k := (1461×ya) ÷ 4+(153×m+2) ÷ 5 + d
end
```

```
procedure KDATE (k,d,m,ya);
integer k,d,m,ya;
comment KDATE converts a serial day number k to the corre-
  sponding calendar date, Gregorian calendar. It computes day d,
  month m, and the last two decimals of the year, ya, without
  using tables. The procedure is valid from k = 1 (1 March 00) to
  k = 36465 (31 December 99) for any one century. For the 20th
  Century the relation between k and theulian day number j
  (at noon) is j = k + 2415079;
begin ya := (4×k−1) ÷ 1461; d := 4×k − 1 − 1461 × ya;
  d := (d+4) ÷ 4; m := (5×d−3) ÷ 153;
    d := 5×d − 3 − 153×m;
  d := (d+5) ÷ 5;
  if m < 10 then m := m + 3
    else begin m := m − 9; ya := ya + 1 end;
end KDATE
```

CERTIFICATION OF ALGORITHM 199 [Z]
CONVERSIONS BETWEEN CALENDAR DATE AND JULIAN DAY NUMBER [Robert G. Tartzen, *Comm. ACM 8* (Aug. 1963), 444].

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Algorithm 199 was translated into JOVIAL J3 and tested on the Philco 2000. Input was generated with a random number generator that produced uniformly distributed dates between the years 1583 and 2583. The results were checked for 50 different dates in that range.

The procedures as written place unnecessary restrictions on some of the parameters. Expressions cannot always be used as inputs to the procedures. Also, the original input to *JDAY*, *JDATE* and *KDAY* will be modified during the operation of the respective procedures. It should also be noted that in many implementations of ALGOL the use of parameters called by name may be more expensive than those called by value. The call by name is a far more powerful tool than is necessary for most of the parameters of these procedures. For these reasons the following changes are suggested:

1. In **procedure** *JDAY*
   change: **integer** *d, m, y, j;*
   to: **value** *d, m, y;* **integer** *d, m, y, j;*
2. In **procedure** *JDATE*
   change: **integer** *j, d, m, y;* to: **value** *j;* **integer** *j, d, m, y;*
3. In **procedure** *KDAY*
   change: **integer** *d, m, ya, k;*
   to: **value** *d, m, ya;* **integer** *d, m, ya, k;*
4. In **procedure** *KDATE*
   change: **integer** *k, d, m, ya;*
   to: **value** *k;* **integer** *k, d, m, ya;*

ALGORITHM 200
NORMAL RANDOM

RICHARD GEORGE*
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* Work supported by United States Atomic Energy Commission.

```
real procedure NORMAL RANDOM (Mean, Sigma n);
  procedure Random;
  real Mean, Sigma;
  integer n;
  comment Random is assumed to be a real procedure which
    generates a random number uniform on the interval (−1, +1).
    The value of n should be greater than 10, in order to approxi-
    mate the normal distribution with accuracy. However, very
    large values of n will increase the running time. The use of
    Mean and Sigma should be obvious. Reference: R. W. Ham-
    ming, Numerical Methods for Scientists and Engineers;
  begin
    integer i; real sum;
    sum := 0;
    for i := step 1 until n do
      sum := sum + Random;
    NORMAL RANDOM := Mean + Sigma × sum × sqrt (3.0/n)
  end NORMAL RANDOM
```

CERTIFICATION OF ALGORITHM 200 [G5]
NORMAL RANDOM

[Richard George, *Comm. ACM 6* (Aug. 1963), 444]

M. C. PIKE (Recd. 3 May 1965)
Statistical Research Unit of the Medical Research Council, U. College Hospital Medical School, London.

Algorithm 200 has the following errors:

(1) The line

```
real procedure NORMAL RANDOM (Mean, Sigma n);
```

should be changed to

```
real procedure NORMAL RANDOM (Random, Mean,
  Sigma, n);
```

(2) The line

```
procedure Random;
```

should be changed to

```
real procedure Random;
```

With these corrections *NORMAL RANDOM* has been run successfully on the ICT Atlas computer with the Atlas ALGOL compiler.

ALGORITHM 201
SHELLSORT

J. BOOTHROYD
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```
procedure Shellsort (a, n); value n; real array a; integer n;
comment a[1] through a[n] of a[1:n] are rearranged in ascending
  order. The method is that of D. A. Shell, (A high-speed sorting
  procedure, Comm. ACM 2 (1959), 30-32) with subsequences
  chosen as suggested by T. N. Hibberd (An empirical study of
  minimal storage sorting, SDC Report SP-982). Subsequences
  depend on m1 the first operative value of m. Here m1 = 2^k - 1
  for 2^k ≤ n < 2^(k+1). To implement Shell's original choice of m1 =
  [n/2] change the first statement to m := n;
begin integer i, j, k, m; real w;
  for i := 1 step i until n do m := 2 × i - 1;
  for m := m ÷ 2 while m ≠ 0 do
    begin k := n - m;
      for j := 1 step 1 until k do
        begin for i := j step -m until 1 do
          begin if a[i+m] ≧ a[i] then go to 1;
            w := a[i]; a[i] := a[i+m]; a[i+m] := w;
          end i;
        1: end j
    end m
end Shellsort;
```

CERTIFICATION OF ALGORITHM 201
SHELLSORT [J. BOOTHROYD, *Comm. ACM 6* (Aug. 1963), 445]

M. A. BATTY (Recd 27 Jan. 1964)
English Electric Co., Whetstone, Nr. Leicester, England

This algorithm has been tested successfully using the DEUCE ALGOL Compiler. When the first statement of the algorithm was replaced by the statement

$$m := n;$$

to implement Shell's original choice of $m_1 := n/2$, a slight increase in sorting time was observed with most of the cases tested.

REMARK ON ALGORITHM 201 [M1]
SHELLSORT [J. Boothroyd, *Comm. ACM 6* (Aug. 1963), 445]

J. P. CHANDLER AND W. C. HARRISON* (Recd. 19 Sept. 1969)
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* This work was supported in part by AEC Contract No. AT-(40-1)-3509. Computational costs were supported in part by National Science Foundation Grant GJ 367 to the Florida State University Computing Center.

KEY WORDS AND PHRASES: sorting, minimal storage sorting, digital computer sorting
CR CATEGORIES: 5.31

Hibbard [1] has coded this method in a way that increases the speed significantly. In SHELLSORT, each stage of each sift consists of successive pair swaps. The modification replaces each set of n pair swaps by one "save," n − 1 moves, and one insertion.

Table I gives timing information for ALGOL, FORTRAN, and COMPASS (assembly language) versions of SHELLSORT and the modified version (called SHELLSORT2), for the CDC 6400 computer. The savings in time achieved by the modification are 32%, 17%, and 21%, respectively. The savings are greater than this when vectors of more than one word each are being sorted.

TABLE I. SORTING TIMES IN SECONDS FOR 10,000 RANDOMLY ORDERED NUMBERS ON THE CDC 6400 COMPUTER

Algorithm	*Source Language*		
	ALGOL	FORTRAN	COMPASS
SHELLSORT	53.40	7.18	2.38
SHELLSORT2	36.56	5.98	1.87

The comparative execution times of the ALGOL and FORTRAN versions, for these compilers, are quite interesting.

REFERENCES:
1. HIBBARD, T. N. An empirical study of minimal storage sorting. *Comm. ACM 6* (May 1963), 206.

ALGORITHM 202
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER

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```
procedure PERLE (S, N, I, E);
integer array S; integer N; Boolean I; label E;
comment If the array S contains a certain permutation of the
  N digits 1, 2, ··· , N before call, the procedure will replace
  this with the lexicographically next permutation. If initializa-
  tion is required set the Boolean variable I equal true, which
  will be changed automatically to false through the first call,
  otherwise set I equal false. If no further permutation can be
  generated, exit will be made to E. For reference see BIT 2
  (1962), 228-231;
begin integer j, u, w;
if I then begin for j = 1 step 1 until N do S[j] := j;
            I := false; go to Rose
          end;
w := N;
Lilie: if S[w] < S[w-1] then
       begin if w = 2 then go to E;
         w := w - 1; go to Lilie
       end;
u := S[w-1];
for j := N step -1 until w do
begin if S[j] > u then
      begin S[w-1] := S[j];
        S[j] := u; go to Tulpe
      end
end;
Tulpe: for j := 0 step 1 until (N-w-1)/2 + 0.1 do
       begin u := S[N-j];
         S[N-j] := S[w+j]; S[w+j] := u
       end;
Rose:
end PERLE
```

CERTIFICATION OF ALGORITHM 202 [G6]
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER

[Mok-Kong Shen, *Comm. ACM 6* (Sept. 1963), 517]

Roger W. Elliott (Recd. 5 May 1965)
The University of Texas, Austin

The equal sign in the second line after the comment should be replaced by a replacement operator. With this minor correction, *PERLE* was translated into Algol for the CDC 1604. The following times for generating all of the $n!$ permutations of a given vector of length n and the following values of $r_n = t_n/nt_{n-1}$ [See *Comm. ACM 5* (Apr. 1962), 209] were observed.

n	5	6	7	8
t_n(sec)	.168	1.01	7.08	56.75
r_n	1.0	1.00	1.00	1.00

REMARKS ON:

ALGORITHM 87 [G6]
PERMUTATION GENERATOR
[John R. Howell, *Comm. ACM 5* (Apr. 1962), 209]
ALGORITHM 102 [G6]
PERMUTATION IN LEXICOGRAPHICAL ORDER
[G. F. Schrak and M. Shimrat, *Comm. ACM 5* (June (1962), 346]
ALGORITHM 130 [G6]
PERMUTE
[Lt. B. C. Eaves, *Comm. ACM 5* (Nov. 1962), 551]
ALGORITHM 202 [G6]
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER
[Mok-Kong Shen, *Comm. ACM 6* (Sept. 1963), 517]

R. J. Ord-Smith (Recd. 11 Nov. 1966, 28 Dec. 1966 and 17 Mar. 1967)
Computing Laboratory, University of Bradford, England

A comparison of the published algorithms which seek to generate successive permutations in lexicographic order shows that Algorithm 202 is the most efficient. Since, however, it is more than twice as slow as transposition Algorithm 115 [H. F. Trotter, Perm, *Comm. ACM 5* (Aug. 1962), 434], there appears to be room for improvement. Theoretically a "best" lexicographic algorithm should be about one and a half times slower than Algorithm 115. See Algorithm 308 [R. J. Ord-Smith, Generation of Permutations in Pseudo-Lexicographic Order, *Comm. ACM 10* (July 1967), 452] which is twice as fast as Algorithm 202.

ALGORITHM 87 is very slow.

ALGORITHM 102 shows a marked improvement.

ALGORITHM 130 does not appear to have been certified before. We find that, certainly for some forms of vector to be permuted, the algorithm can fail. The reason is as follows.

At execution of $A[f] := r$; on line prior to that labeled *schell*, f has not necessarily been assigned a value. f has a value if, and only if, the Boolean expression $B[k] > 0 \wedge B[k] < B[m]$ is **true** for at least one of the relevant values of k. In particular when matrix A is set up by $A[i] := i$; for each i the Boolean expression above is **false** on the first call.

ALGORITHM 202 is the best and fastest algorithm of the exicographic set so far published.

A collected comparison of these algorithms is given in Table I. t_n is the time for complete generation of $n!$ permutations. Times are scaled relative to t_8 for Algorithm 202, which is set at 100. Tests were made on an ICT 1905 computer. The actual time t_8 for Algorithm 202 on this machine *was* 100 seconds. r_n has the usual definition $r_n = t_n/(n \cdot t_{n-1})$.

TABLE I

Algorithm	t_6	t_7	t_8	r_6	r_7	r_8
87	118	—	—	—	—	—
102	2.1	15.5	135	1.03	1.08	1.1
130	—	—	—	—	—	—
202	1.7	12.4	100	1.00	1.00	1.00

ALGORITHM 203
STEEP1

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N. V. Philips' Gloeilampenfabrieken
Eindhoven-Netherlands

```
procedure STEEP1 (lb, xs, ub, dx, xmin, fmin, n, eps, relax, dxmax,
  eta, psi, pmax, zeta, FUNK);
value dx, n, eps, relax, dxmax, eta, psi, pmax, zeta;
integer n;
real fmin, eps, relax, dxmax, eta, psi, pmax, zeta;
array lb, xs, ub, dx, xmin; real procedure FUNK;
comment STEEP1 is a subroutine to find the minimum of a
  differentiable function of n variables, using the method of
  steepest descent. It mainly consists of three parts: (1) a sub-
  routine ATIVE, for computing the partial derivatives, (2) a
  subroutine STEP, for computing the components of an array
  xstep[1:n], which is a new approximation of xmin[1:n], (3) the
  compound tail of the procedure body. Both subroutines are
  only called for once, but by writing the program in this way it
  is quite easy to change the flow of the program.
    Significance of the parameters: lb(i), ub(i) are lower and
  upper bounds for the independent variables. xs(i) is the starting
  value for xmin(i). xmin(i) is the computed ith component of
  the minimum, fmin the value of the function in xmin. n is the
  number of variables. eps is a small number which is a measure
  of the desired accuracy—rather of fmin than of xmin(i). FUNK
  (x) is the function to be minimized. The other parameters are
  described in the comments on the three parts mentioned;
begin integer j; real alpha, p; array xstep, dfdx, dfpr[1:n];
procedure ATIVE;
begin real beta, gamma, lambda; Boolean A, B;
comment 1. A useful estimate for the derivative is
  (f(x+dx)-f(x-dx))/2dx, where dx should be small, but not so small
  that roundoff noise dominates. This may be achieved by taking
  dx such that eta < |(f(x+dx)-f(x-dx))/f(x)| < 100 eta, where eta is
  a measure for the relative roundoff error. When |f(x)| < 1 it is
  better to replace the denominator by a constant. In the program
  the parameter psi is used for this purpose. The components
  dx(i) are used as a first guess. When the derivative is 0, the
  program enlarges dx until dx > dxmax.
ATIVE computes dfdx[1:n] in xmin. The previously computed
  partial derivatives dfpr[1:n] as well as relax are used for relaxa-
  tion purposes. See comment 3. The Boolean A is used when
  x+dx or x-dx crosses the boundary ub or lb. In that case fmin
  has to be recomputed afterwards. The Boolean B is of a some-
  what complicated nature. It may be seen that dx has the char-
  acter of an own array for ATIVE. In the neighborhood of the
  minimum this may have the following effect: A step in one
  variable is taken such that f(x+dx) becomes equal to f(x-dx).
  Then in the next call for ATIVE dx has to be doubled, etc. By
  using the Boolean B it is possible to keep dx constant near the
  minimum.
    A similar effect may occur in the large. When f(x) tends to a
  constant for x tending to +∞ and -∞, then for |x| large dx
  has to be taken large. It is only possible to make dx smaller in
  the neighborhood of the minimum by reducing dx after each
  call of ATIVE.
    From the last two remarks one may deduce that the first
  guess for dx(i) should be made with considerable care. Tabulat-
  ing the function near the starting point may be very helpful;
begin ATIVE: lambda := 0;
for j := 1 step 1 until n do
begin
large: A := B := false; if xmin[j] + dx[j] > ub[j]
    then begin xmin[j] := ub[j] - dx[j]; A := true end
      else if xmin[j] - dx[j] < lb[j]
    then begin xmin[j] := lb[j] + dx[j]; A := true end;
small: xmin[j] := xmin[j] + dx[j]; alpha := FUNK (xmin);
    xmin[j] := xmin[j] - 2 × dx[j]; beta := FUNK (xmin);
    xmin[j] := xmin[j] + dx[j]; if A then fmin := FUNK
      (xmin);
    A := false;
    if alpha - fmin > 0 ∧ beta - fmin > 0
    then begin B := true; go to comp end;
    gamma := abs((alpha-beta)/(if abs(fmin) < psi then
      psi else fmin));
    if gamma > 100 × eta then
      begin dx[j] := .2 × dx[j]; go to small end;
    if gamma < eta then
      begin dx[j] := 2 × dx[j]; if dx[j] < dxmax then
      go to large else dx[j] := dxmax end
    comp: dfdx[j] := (alpha-beta)/(2 × dx[j]);
      lambda := lambda + dfdx[j] ↑ 2;
      if ¬ B then dx[j] := .5 × dx[j]
  end for; lambda := sqrt (lambda);
  for j := 1 step 1 until n do
    dfdx[j] := dfdx[j]/lambda
  end procedure ATIVE;

procedure STEP;
comment 2. A step is taken in all variables at the same time.
  The order of magnitude of the step in one variable should be
  of the order of magnitude of this variable. To accomplish this
  three weighting factors are given to the partial derivatives:
  1) λ = (Σ_{i=1}^{n} (∂f/∂x_i)^2)^{-½} (see subroutine ATIVE),
  2) |x_i|, or when small, zeta,
  3) a number p, which is put equal to 1 at the beginning of the
     program and which tends to 0 at the minimum.
  After a decrease of the function the step is accepted and p is
  multiplied by 1.5. After an increase p is divided by 2. pmax
  replaces p when p becomes greater than pmax;
begin for j := 1 step 1 until n do
begin alpha := (1-relax) × dfdx[j] + relax × dfpr[j];
  xstep[j] := xmin[j] - p × alpha ×
  (if abs(xmin[j]) < zeta then zeta else abs(xmin[j]));
  dfpr[j] := alpha;
  if xstep[j] > ub[j] then xstep[j] := ub[j]
else if xstep[j] < lb[j] then xstep[j] := lb[j]
end for
end STEP;
```

comment 3. In the next part—the compound tail—the calls for *ATIVE* and *STEP* are organized. The values 1.5 and .5 of the factors of p are not very important. During the iteration p gets an optimal value, which slowly varies. Only at the end p rapidly tends to 0. The programme was tested on the functions $\frac{y^2+1}{x^2+1}$ and $\frac{(x-y)^2-2}{(x+y)^2+2}$, the latter being the first one except for a rotation of the xy-plane over $\pi/4$ radians. In the first case a "gutter" coincides with the x-axis, while for $x > 0$ and $|y| \geqslant 1$ $\frac{\partial f}{\partial x} \leqslant 0$. In the second case, where the gutter is along the line $x=y$, the relaxation is especially interesting, because with *relax* = 0 (and *pmax*=100) the iteration follows the gutter in an unstable way. With starting values $x=-14$ and $y=21$ from $x=y=26$ about 300 steps were taken along the gutter with p about .01. With *relax* = .35 and *pmax* = .5 we had about 150 steps from $x=y=23$. In the gutter itself *relax* = .85 gave the best results, but in that case the gutter was reached at $x=y=63$.

Other parameter values were: *zeta* = *psi* = 1, *dxmax*=100, *eta* = 10^{-7} with *eps* = 10^{-8} gave *fmin* in 10 figures correctly and *xmin*[*i*] in 4 to 6 figures for various starting values of *xs*[*i*];

```
p := 1;
for j := 1 step 1 until n do
begin xmin[j] := xs[j]; dfpr[j] := 0 end; fmin := FUNK
  (xmin);
deriv: ATIVE;
next: STEP;
      alpha := FUNK (xstep);
if alpha < fmin then
  begin fmin := alpha; p := 1.5 × p;
        if p > pmax then p := pmax;
        for j := 1 step 1 until n do xmin[j] := xstep[j];
        go to deriv end;
p := .5 × p;
if p > eps then go to next;
comment As p has become smaller than eps this is the end of
  STEEP1. The program ATIVE takes up rather a lot of computer
  time by the way it chooses a value for dx(i). A thorough simpli-
  fication is obtained by taking dx(i) as 10↑ − 3 × abs(xmin[i]),
  where again xmin[i] may be replaced by zeta. Further, at the
  cost of some loss of accuracy, computing time is saved by taking
  (f(x+h)−f(x))/h as an estimate for the derivative. This program,
  as far as it differs from STEEP1, is described in algorithm 204,
  STEEP2. An interesting compromise between the two methods
  is obtained by interchanging the computation of dx and dfdx in
  ATIVE of STEEP1 and omitting the iteration on dx. This
  routine ATIVE, which has to be used in STEEP1, is given by
  J. G. A. Haubrich in algorithm 205;
end STEEP1
```

CERTIFICATION OF ALGORITHM 203 [E4]
STEEP1 [E. J. Wasscher, *Comm. ACM 9* (Sept. 1963), 517]

PHILIP WALLACK (Recd. 25 May 1964)
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STEEP1 was translated into FORTRAN IV and run on the IBM 7094. The program was tested on the function $x^4 + y^4 - 1$, with starting values $x = y = 1.5$. Other parameter values were those suggested in the body of the algorithm. After 17 steps the values of the variables were $x = .0180$, $y = .0191$, and the function value *fmin* = −.9999999.

I feel that good programming practice requires that a count be kept of the number of steps taken in *STEEP1* and the number of iterations in *ATIVE*, with running checks on both these quantities to control looping. Counters were set up for this purpose in the version of the program I ran.

CERTIFICATION OF ALGORITHM 203 [E4]
STEEP1 [E. J. Wasscher, *Comm. ACM 6* (Sept. 1963), 517; *Comm. ACM 7* (Oct. 1964), 585]

J. M. VARAH (Recd. 30 July 1964)
Computation Center, Stanford University, Stanford, Calif.

Algorithm 203 was run on the B5000 at Stanford with the necessary modifications for Burroughs' Extended ALGOL. After some testing, the following errors were found.

1. There is an extra **begin** in procedure *ATIVE*. The first statement after the comment in this procedure should be changed from

```
begin ATIVE: lambda := 0;
```

to

```
lambda := 0;
```

[It was the author's original intention that this **begin** be not in bold-face but that it should be part of the label *begin ATIVE* inserted to clarify the program.—Ed.]

Also, there is a missing semicolon in procedure *ATIVE* at the end of the line preceding *comp*: and procedure *STEP* has an unnecessary **begin-end** block.

2. Because the domain of definition of the function *FUNK* is bounded by the rectangular hyperbox $lb[j] \leqq x[j] \leqq ub[j]$, $j = 1, 2, \cdots, n$, before giving a new direction in which to proceed, the value of *xmin* is checked (in *ATIVE*, under *large*:). If, for any j, *xmin*[j] is within *dx*[j] of the boundary, *xmin*[j] is changed so that it is exactly *dx*[j] from the boundary. However, if the minimum value of *FUNK* occurs at just such a place (say right at the boundary), then a step will be made from this new position back to the boundary. Then the new *xmin*[j] will again be within *dx*[j] of the boundary, so it is moved away, and so on forming a loop. To correct this, the old value of *xmin*[j] should be saved (in *xstep*[j], for example) and below, when *A* is tested, the function value set equal to the minimum of values at *xmin* and *xstep*. The author, when *A* was true (i.e. when such a shift had been made), merely set the function equal to the value at *xmin*.

Specifically, this means changing the lines following *large*: to

```
A := B := false; if xmin[j] + dx[j] > ub[j] then
begin
  xstep[j] := xmin[j];
  xmin[j] := ub[j] − dx[j]; A := true
end
else if xmin[j] − dx[j] < lb[j] then
begin
  xstep[j] := xmin[j];
  xmin[j] := lb[j] + dx[j]; A := true
end;
```

and the conditional statement involving *A* (3rd line after *small*:) to

```
if A then
begin
  gamma := FUNK(xmin);
  if fmin ≦ gamma then xmin[j] := xstep[j]
  else fmin := gamma
end;
```

3. Also in *ATIVE*, under *comp*:, the derivative approximations are all normalized after the **for** loop by division by *lambda*. However, *lambda* will be zero if all *dfdx*[j] are zero to working accuracy. So we should only divide by *lambda* when it is not zero.

Specifically, this means inserting the line

if *lambda* $\neq$ 0 **then**

before the third line from the end of procedure *ATIVE*.

With these corrections, the algorithm did run successfully. It should also be mentioned that procedures *ATIVE* and *STEP* could just as well be blocks with labels *ATIVE* and *STEP* rather than procedures, with the calls on them changed to **go to** *ATIVE* and **go to** *STEP*.

ALGORITHM 204
STEEP2
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```
procedure STEEP2 (lb, xs, ub, dx, xmin, fmin, n, eps, relax
  dxmax, pmax, zeta, FUNK);
value dx, n, eps, relax, dxmax, pmax, zeta;
integer n;
real dx, fmin, eps, relax, dxmax, pmax, zeta;
array lb, xs, ub, xmin; real procedure FUNK;
comment dx should now be taken about 10↑ − 3, dxmax could
  be taken equal to 1. As the program is equal to STEEP1 after
  the declaration of the procedure ATIVE, the ALGOL description
  is cut off there;
begin integer j; real alpha, p;
  array xstep, dfdx, dfpr [1:n];
procedure ATIVE;
begin real beta, lambda; lambda := 0;
  for j := 1 step 1 until n do
begin alpha := dx × (if abs(xmin[j]) < dxmax
  then dxmax else abs (xmin[j]));
  if xmin[j] + alpha > ub[j] then alpha := −alpha;
  xmin[j] := xmin[j] + alpha; beta := FUNK (xmin);
  xmin[j] := xmin[j] − alpha;
  dfdx[j] := (beta − fmin)/alpha;
  lambda := lambda + dfdx[j] ↑2
end for; lambda := sqrt (lambda);
  for j := 1 step 1 until n do dfdx[j] := dfdx[j]/lambda;
end procedure ATIVE
```

ALGORITHM 205
ATIVE
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Eindhoven-Netherlands

```
procedure ATIVE;
begin real beta, lambda; Boolean A;
comment This routine may replace ATIVE in STEEP1. The
  significance of eta has slightly changed;
lambda := 0;
for j := 1 step 1 until n do
begin A := false; alpha := dx[j];
if xmin[j] + alpha > ub[j] then
begin xmin[j] := ub[j] - alpha; A := true end
else if xmin[j] - alpha < lb[j] then
begin xmin[j] := lb[j] + alpha; A := true end;
      xmin[j] := xmin[j] + dx[j]; alpha := FUNK(xmin);
      xmin[j] := xmin[j] - 2 × dx[j]; beta := FUNK(xmin);
      xmin[j] := xmin[j] + dx[j]; if A then fmin := FUNK
        (xmin);
      dfdx[j] := (alpha-beta)/(2 × dx[j]);
      lambda := lambda+dfdx[j] ↑2;
if alpha - fmin > 0 ∧ beta - fmin > 0 then go to end;
beta := abs((alpha-beta)/(if abs(fmin)<psi then psi else fmin));
if beta > eta then dx[j] := .3 × dx[j] else
begin dx[j] := × d3x[j]; if dx[j] > dxmax then dx[j]: = dxmax end;
end: end for;
lambda := sqrt (lambda);
for j := 1 step 1 until n do dfdx[j] := dfdx[j]/lambda
end procedure ATIVE
```

REMARK ON ALGORITHM 205 [E4]
ATIVE [J. G. A Haubrich, *Comm. ACM 6* (Sept. 1963), 519]
E. J. WASSCHER (Recd. 23 Nov. 1964)
Philips Computer Center, N. V. Philips' Gloeilampenfabrieken, Eindhoven, Netherlands

There is a misprint in this Algorithm. The first statement in the fifth line from the end of the procedure *ATIVE* should read:

```
dx[j] := 3 × dx[j];
```

ALGORITHM 206
ARCCOSSIN

MISAKO KONDA
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```
procedure ARCCOSSIN(x) Result:(arccos, arcsin);
value x;
real x, arccos, arcsin;
comment This procedure computes arccos(x) and arcsin(x) for
  -1≦x≦1. The constant 2^-π depends on the word length and
  relative machine precision, and may be replaced by a variable
  identifier. Alarm is the procedure which messages that x is in-
  valid.
  The approximation formula used here was coded for MUSA-
  SINO-1 in its own language at the Electrical Communication
  Laboratory Tokyo. This algorithm was translated into FAP and
  successfully ran on an IBM 7090;
begin real A, x1, x2, a; integer r;
  if abs(x) > 1
  then go to Alarm
  else if abs(x) > 2↑ (-27)
    then go to L1
    else begin arccos := 1.5707963; go to L3
      end;
L1: if x = 1
    then begin arccos := 0; go to L3
      end
    else if x = - 1
      then begin arccos := 3.1415926; go to L3
        end
      else begin A := 0; x1 := x;
          for r := 0 step 1 until 26 do
          begin if x1<0
            then begin a := 1; x2 := 1-2 × x1 ↑2 end
            else begin a := 0; x2 := 2 × x1 ↑2 - 1 end;
            A := A + a × 2 ↑(-r-1);
            x1 := x2
          end;
        arccos := 3.1415926 × A;
        end;
L3: arcsin := 1.570963 - arccos;
    end ARCCOSSIN
```

Results were obtained for a selection of values of the argument between 0 and 1. Accuracy is about 7+ decimal digits over the entire range, by comparison with the tables of inverse sines in [*Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series #55, U.S. Government Printing Off., Washington, D.C., June 1964, 203-212]. Average execution time was 43 milliseconds.

The efficiency of the procedure could be significantly improved by avoiding the computation of $a \times 2\uparrow(-r-1)$. Powers of 0.5 may be accumulated within the loop, and the modification of A may be skipped entirely when $a = 0$. Actually, if efficiency is important, procedures using the intrinsic *arctan* and the common trigonometric identities are preferable. Such routines, on the B-5000, give full machine accuracy (11+ significant figures) in about 2 milliseconds execution time.

REMARK ON ALGORITHM 206 [B1]
ARCCOSSIN [Misako Konda, *Comm. ACM 6* (Sept. 1963), 519]

HENRY J. BOWLDEN (Recd. 30 Sept. 1964 and 5 Nov. 1964)
Westinghouse Electric Corp., R&D Ctr., Pittsburgh, Pa.

Algorith ı 206 was transcribed into Burroughs Extended ALGOL after correcting one typographical error, namely the value of $\pi/2$ in the statement labeled *L3*, which should be 1.5707963.

ALGORITHM 207
STRINGSORT

J. BOOTHROYD
English Electric-Leo Computers, Ltd.
Staffordshire, England

```
procedure stringsort (a, n); comment elements a[1] ··· a[n]
  of a[1:2n] are sorted into ascending sequence using a[n+1] ···
  a[2n] as auxiliary storage. Von Neumann extended string logic
  is employed to merge input strings from both ends of a sending
  area into output strings which are sent alternately to either
  end of a receiving area. The procedure takes advantage of
  naturally occurring ascending or descending order in the origi-
  nal data;
value n; integer n; array a;
begin integer d, i, j, m, u, v, z; integer array c[−1:1];
  switch p := jz1, str i; switch q := merge, jz2;
oddpass: i := 1; j := n; c[−1] := n + 1; c[1] := 2 × n;
allpass: d := 1; go to firststring;
merge: if a[i] ≧ a[z]
       then begin go to p[v];
         jz1: if a[j] ≧ a[z]
              then ij: begin if a[i] ≧ a[j]
                             then str j: begin a[m] := a[j];
                               j := j − 1 end
                             else str i: begin a[m] := a[i];
                               i := i + 1 end
                       end
              else begin v := 2; go to str i end
         end
       else begin u := 2;
           jz2: if a[j] ≧ a[z]
                then go to str j
                else begin d := −d; c[d] := m;
                       firststring: m := c[−d];
                         v := u := 1;
                       go to ij
                     end
            end;
z := m; m := m + d; if j ≧ i then go to q[u];
if m > n + 1 then begin comment evenpass; i := n + 1;
                  j := 2 × n; c[−1] := 1; c[1] := n; go to
                  allpass end
             else if m < n + 1 then go to oddpass
end stringsort;
```

Number of Items	*Time in Seconds*
10	0.03
20	0.05
50	0.20
100	0.38
200	1.03
500	3.22
1000	6.43
2000	12.85
5000	38.72
10000	90.72

CERTIFICATION OF ALGORITHM 207 [M1]
STRINGSORT [J. Boothroyd, *Comm. ACM 6* (Oct. 1963), 615]

CHARLES R. BLAIR (Recd. 31 Jul. 1964)
Department of Defense, Washington 25, D. C.

STRINGSORT compiled and ran successfully without correction on the ALDAP translator for the CDC 1604A. The following sorting times were observed.

ALGORITHM 208
DISCRETE CONVOLUTION

WILLIAM T. FOREMAN, JR.
Collins Radio Co.
Newport Beach, Calif.

```
procedure Discrete Convolution (m, n, prs) result: (Conv);
integer m, n; real procedure prs; real array conv;
comment This procedure finds the probability distribution of
  the sum of m independent variables, each with a known distribu-
  tion over the nonnegative integers. A real procedure prs with
  results pr[k] is assumed to find each probability distribution in
  succession. The maximum sum for which probabilities are
  computed must be fixed by the user. The number of iterations
  is roughly m²n/2. The procedure prs will in general depend on
  additional parameters and should include the read-in of the
  parameters for that distribution. It may include the selection
  of one function from a set;
begin integer i, j, k, ix1, ix2;
real array prob [1:2, 0:m], pr[0:m];
i := 1; ix1 := 1; ix2 := 2; prs (m) result: (pr);
for j := 0 step 1 until m do prob[ix1, j] := pr[j];
for i := 2 step 1 until n do
  begin
    if ix1 = 1 then begin ix2 := 1; ix1 := 2 end
      else begin ix2 := 2; ix1 := 1 end
    prs (m) result: (pr);
    for j := 0 step 1 until m do
    begin
      prob[ix1, j] := 0;
      for k := 0 step 1 until j do
        prob[ix1, j] := prob[ix1, j] + pr[k] × prob[ix2, j−k]
    end j
  end i;
for j := 0 step 1 until m do conv[j] := prob[ix1, j]
end Discrete Convolution
comment The convolution of discrete probability series is
  isomorphic to the multiplication of polynomials. A useful vari-
  ation is to omit the parameters i, n and have prs recognize
  the end of input. A FORTRAN program using this procedure has
  been run on the IBM 7090 to find the sum of queue lengths in a
  teletype switching center, where messages arrived according
  to the Poisson distribution and message lengths were distributed
  negative-exponentially. The following was used as the prob-
  ability procedure;
procedure prs (m) result: (pr);
value m; procedure read;
real array pr; integer m;
begin real trafficrate, linespeed, rho; integer j;
  read (trafficrate, linespeed);
  rho := trafficrate/linespeed;
  pr[0] : 1 − rho;
  for j := 1 step until m do pr[j] := rho × pr[j−1]
end prs
```

ALGORITHM 209
GAUSS

D. IBBETSON,
Elliott Brothers (London) Ltd.,
Elstree Way, Borehamwood, Herts., England

```
real procedure Gauss(x); value x; real x;
comment Gauss calculates (1/√(2π)) ∫ from -∞ to x of exp(-½u²) du by means
  of polynomial approximations due to A. M. Murray of Aberdeen
  University;
begin real y, z, w;
  if x = 0 then z := 0
  else
  begin y := abs(x)/2;
    if y ≧ 3 then z := 1
    else if y < 1 then
    begin w := y × y;
      z := (((((((0.000124818987 × w
        -0.001075204047) × w +0.005198775019) × w
        -0.019198292004) × w +0.059054035642) × w
        -0.151968751364) × w +0.319152932694) × w
        -0.531923007300) × w +0.797884560593) × y × 2
    end
    else
    begin y := y - 2;
      z := ((((((((((((-0.000045255659 × y
        +0.000152529290) × y -0.000019538132) × y
        -0.000676904986) × y +0.001390604284) × y
        -0.000794620820) × y -0.002034254874) × y
        +0.006549791214) × y -0.010557625006) × y
        +0.011630447319) × y -0.009279453341) × y
        +0.005353579108) × y -0.002141268741) × y
        +0.000535310849) × y +0.999936657524
    end
  end;
  Gauss := if x > 0 then (z+1)/2 else (1-z)/2
end Gauss;
```

CERTIFICATION OF ALGORITHM 209
GAUSS [D. Ibbetson, *Comm. ACM 6* (Oct. 1963), 616]

(Pvt.) G. W. GLADFELTER (Recd 4 Nov. 63)
RA17667701, 1st Inf. Battle Group U.S. Military Academy (9822), West Point, N.Y.

The algorithm was translated into FORTRAN for the GE 225 and used to publish a table of the error function. No errors were found in the algorithm and the table produced agreed with the published tables at hand (6 significant figures).

CERTIFICATION OF ALGORITHM 209 [S15]
GAUSS [D. Ibbetson, *Comm. ACM 6*, Oct. 1963, 616]

M. C. PIKE
Statistical Research Unit of the Medical Research Council, University College Hospital Medical School, London, England

This procedure was tested on an Elliott 803 computer using the standard Elliott ALGOL compiler. The expression

$$2 \times Gauss\ (x) - 1$$

was evaluated for $x = 0(.01)6$ and the answers checked with those given in *Tables of Probability Functions, vol. II*, U.S. National Bureau of Standards, Washington, D.C., 1942, where they are given to 15 decimal places. There was a maximum error of 1 in the 8th decimal place.

REMARKS ON:
ALGORITHM 123 [S15]
REAL ERROR FUNCTION, ERF(x)

[Martin Crawford and Robert Techo *Comm. ACM 5* (Sept. 1962), 483]

ALGORITHM 180 [S15]
ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 314]

ALGORITHM 181 [S15]
COMPLEMENTARY ERROR FUNCTION—LARGE X

[Henry C. Thacher Jr. *Comm. ACM 6* (June 1963), 315]

ALGORITHM 209 [S15]
GAUSS

[D. Ibbetson. *Comm. ACM 6* (Oct. 1963), 616]

ALGORITHM 226 [S15]
NORMAL DISTRIBUTION FUNCTION

[S. J. Cyvin. *Comm. ACM 7* (May 1964), 295]

ALGORITHM 272 [S15]
PROCEDURE FOR THE NORMAL DISTRIBUTION FUNCTIONS

[M. D. MacLaren. *Comm. ACM 8* (Dec. 1965), 789]

ALGORITHM 304 [S15]
NORMAL CURVE INTEGRAL

[I. D. Hill and S. A. Joyce. *Comm. ACM 10* (June 1967), 374]

I. D. HILL AND S. A. JOYCE (Recd. 21 Nov. 1966)
Medical Research Council,
Statistical Research Unit, 115 Gower Street, London W.C.1., England

These algorithms were tested on the ICT Atlas computer using the Atlas ALGOL compiler. The following amendments were made and results found:

ALGORITHM 123

(i) **value** x; was inserted.

(ii) $abs(T) < {}_{10}-10$ was changed to $Y - T = Y$

both these amendments being as suggested in [1].

(iii) The labels 1 and 2 were changed to *L*1 and *L*2, the **go to** statements being similarly amended.
(iv) The constant was lengthened to 1.12837916710.
(v) The extra statement $x := 0.707106781187 \times x$ was made the first statement of the algorithm, so as to derive the normal integral instead of the error function.

The results were accurate to 10 decimal places at all points tested except $x = 1.0$ where only 2 decimal accuracy was found, as noted in [2]. There seems to be no simple way of overcoming the difficulty [3], and any search for a method of doing so would hardly be worthwhile, as the algorithm is slower than Algorithm 304 without being any more accurate.

ALGORITHM 180
(i) $T := -0.56418958/x/exp(v)$ was changed to $T := -0.564189583548 \times exp(-v)/x$. This is faster and also has the advantage, when v is very large, of merely giving 0 as the answer instead of causing overflow.
(ii) The extra statement $x := 0.707106781187 \times x$ was made as in (v) of Algorithm 123.
(iii) **for** $m := m + 1$ was changed to **for** $m := m + 2$. $m+1$ is a misprint, and gives incorrect answers.

The greatest error observed was 2 in the 11th decimal place.

ALGORITHM 181
(i) Similar to (i) of Algorithm 180 (except for the minus sign).
(ii) Similar to (ii) of Algorithm 180.
(iii) m was declared as **real** instead of **integer**, as an alternative to the amendment suggested in [4].

The results were accurate to 9 significant figures for $x \leqslant 8$, but to only 8 significant figures for $x = 10$ and $x = 20$.

ALGORITHM 209
No modification was made. The results were accurate to 7 decimal places.

ALGORITHM 226
(i) $10 \uparrow m/(480 \times sqrt(2 \times 3.14159265))$ was changed to $10 \uparrow m \times 0.000831129750836$.
(ii) **for** $i := 1$ **step** 1 **until** $2 \times n$ **do** was changed to $m := 2 \times n$; **for** $i := 1$ **step** 1 **until** m **do**.
(iii) $-(i \times b/n) \uparrow 2/8$ was changed to $-(i \times b/n) \uparrow 2 \times 0.125$.
(iv) **if** $i = 2 \times n - 1$ was changed to **if** $i = m - 1$
(v) $b/(6 \times n \times sqrt(2 \times 3.14159265))$ was changed to $b/(15.0397696478 \times n)$.

Tests were made with $m = 7$ and $m = 11$ with the following results:

x	*Number of significant figures correct*		*Number of decimal places correct*	
	$m = 7$	$m = 11$	$m = 7$	$m = 11$
−0.5	7	11	7	11
−1.0	7	10	7	10
−1.5	7	10	8	10
−2.0	7	9	8	10
−2.5	6	9	8	11
−3.0	6	7	8	9
−4.0	5	7	10	11
−6.0	2	1	12	10
−8.0	0	0	11	9

Perhaps the comment with this algorithm should have referred to decimal places and not significant figures. To ask for 11 significant figures is stretching the machine's ability to the limit, and where 10 significant figures are correct, this may be regarded as acceptable.

ALGORITHM 272
The constant .99999999 was lengthened to .9999999999.

The accuracy was 8 decimal places at most of the points tested, but was only 5 decimal places at $x = 0.8$.

ALGORITHM 304
No modification was made. The errors in the 11th significant figure were:

abs(*x*)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
0.5	1	1
1.0	1	2
1.5	21[a](5)	2
2.0	25[a](0)	4
3.0	0	0
4.0	2	3
6.0	6	0
8.0	14	0
10.0	23	0
20.0	35	0

[a] Due to the subtraction error mentioned in the comment section of the algorithm. Changing the constant 2.32 to 1.28 resulted in the figures shown in brackets.

To test the claim that the algorithm works virtually to the accuracy of the machine, it was translated into double-length instructions of Mercury Autocode and run on the Atlas using the EXCHLF compiler (the constant being lengthened to 0.39894228040143267793994 6). The results were compared with hand calculations using Table II of [5]. The errors in the 22nd significant figure were:

abs(*x*)	$x > 0 \equiv upper$	$x > 0 \not\equiv upper$
1.0	2	3
2.0	7	1
4.0	2	0
8.0	8	0

Timings. Timings of these algorithms were made in terms of the Atlas "Instruction Count," while evaluating the function 100 times. The figures are not directly applicable to any other computer, but the relative times are likely to be much the same on other machines.

INSTRUCTION COUNT FOR 100 EVALUATIONS

abs(x)	Algorithm number							
	123	180	181	209	226 $m = 7$	272	304[a]	304[b]
0.5	58			8	97	24	25	24
1.0	65[c]			8	176	24	29	29
1.5	164	128	127	9	273	25	35	35
2.0	194	78	90	8	387	24	39	39
2.5	252	54	68	10	515	24	131	44
3.0		42	51	9	628	25	97	50
4.0		27	39	9	900[d]	25	67	44
6.0		15	30	6	1400[d]	16	49	23
8.0		9	28	7	2100[d]	18	44	11
10.0		10	25	5	2700[d]	16	38	11
20.0		9	22	5	6500[d]	16	32	11
30.0		9	9	5	10900[d]	16	11	11

[a] Readings refer to $x > 0 \equiv$ *upper*.
[b] Readings refer to $x > 0 \not\equiv$ *upper*.
[c] Time to produce incorrect answer. A count of 120 would fit a smooth curve with surrounding values.
[d] 100 times Instruction Count for 1 evaluation.

Opinion. There are advantages in having two algorithms available for normal curve tail areas. One should be very fast and reasonably accurate, the other very accurate and reasonably fast. We conclude that Algorithm 209 is the best for the first requirement, and Algorithm 304 for the second.

Algorithms 180 and 181 are faster than Algorithm 304 and may be preferred for this reason, but the method used shows itself in Algorithm 181 to be not quite as accurate, and the introduction of this method solely for the circumstances in which Algorithm 180 is applicable hardly seems worth while.

Acknowledgment. Thanks are due to Miss I. Allen for her help with the double-length hand calculations.

REFERENCES:

1. THACHER, HENRY C. JR. Certification of Algorithm 123. *Comm. ACM 6* (June 1963), 316.

2. IBBETSON, D. Remark on Algorithm 123. *Comm. ACM 6* (Oct. 1963), 618.

3. BARTON, STEPHEN P., AND WAGNER, JOHN F. Remark on Algorithm 123. *Comm. ACM 7* (Mar. 1964), 145.

4. CLAUSEN, I., AND HANSSON, L. Certification of Algorithm 181. *Comm. ACM 7* (Dec. 1964), 702.

5. SHEPPARD, W. F. *The Probability Integral.* British Association Mathematical Tables VII, Cambridge U. Press, Cambridge, England, 1939.

ALGORITHM 210
LAGRANGIAN INTERPOLATION

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* Undergraduate research project, Computer Science Program, Univ. of Dayton.

```
procedure LAGRANGE (N, u, X, Y, ANS); real array X, Y;
  integer N; real u, ANS;
comment This procedure evaluates an Nth degree Lagrange
  polynomial, given N + 1 data coordinates, and u the value
  where interpolation is desired. X is the abscissa array and Y
  the ordinate array. ANS is the resultant value of the function
  at u. The notation is that used in R. W. Hamming, Numerical
  Methods for Scientists and Engineers, pp. 94-95 (McGraw-Hill
  Book Company, Inc., 1962);
begin integer i, j; real L;
  ANS := 0.0;
  for j := step 1 until N+1 do
begin L := 1.0;
  for i := step 1 until N+1 do
begin if i ≠ j then L := L × (u-X[i])/(X[j]-X[i])
end;
  ANS := ANS + L × Y[j]
end end
```

ALGORITHM 211
HERMITE INTERPOLATION

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* Undergraduate research project, Computer Science Program, Univ. of Dayton.

```
procedure HERMITE (n, u, X, Y, Y1, ANS); real array X, Y,
    Y1;
  integer n; real u, ANS;
comment This procedure evaluates a(2n+1)th degree Hermite
  polynomial, given the value of the function and its first deriva-
  tive at each of n + 1 points. X is the abscissa array, Y the
  ordinate array, and Y1 the derivative array. ANS is the interpo-
  lated value of the function at u. REFERENCE: R. W. Hamming,
  Numerical Methods for Scientists and Engineers, pp. 96-97 (Mc-
  Graw-Hill Book Company, Inc., 1962);
begin integer i, j; real h, a;
  ANS := 0.0;
  for j := 1 step 1 until n + 1 do
begin h := 1.0; a := 0.0;
  for i := 1 step 1 until n + 1 do
begin if i = j then go to out;
  h := h × (u-X[i])↑2/(X[j]-X[i])↑2;
  a := a + 1.0/(X[j]-X[i]);
out: end;
  ANS := ANS + h × ((X[j]-u)×(2×a×Y[j]-Y1[j])+Y[j])
end end
```

CERTIFICATION OF ALGORITHM 211
HERMITE INTERPOLATION [George R. Schubert, *Comm. ACM*, Oct. 1963]

THOMAS A. DWYER
Argonne National Laboratory, Argonne, Ill.

The body of *HERMITE* was transcribed for the Dartmouth SCALP processor for the LGP-30 computer and ran successfully without corrections. It was tested using the error function and its derivatives. Roundoff error in the LGP-30 began to appear for values of n greater than 3. For n equal to 2 (third degree polynomial) the interpolated value agreed with the function within machine limitations (six significant figures) for steps in the argument data of 0.005.

ALGORITHM 212
FREQUENCY DISTRIBUTION
MALCOLM D. GRAY
The Boeing Co., Seattle, Wash.

```
procedure FREQUENCY (N, A, B, IUL, K, X, KA);
integer N, IUL; integer array KA; real A, B, K;
real array X;
comment Given a set X of variables in some interval I = [a, b]
  such that a ≦ min x, max x ≦ b, FREQUENCY determines the
  frequency distribution of X over k equal, half open subintervals
  of I. The interval I is transformed to the interval J = [0, k]
  with unit subintervals by x' = (x_i−a)/[(b−a)/k], i = 1, 2, ···,
  n, and considering x' = L × M, L and M integers. The value
  L then immediately determines the subinterval and M is used
  for boundary points. If IUL = 0, the subintervals are open
  on the upper end, except the kth. On entry, the array KA is
  assumed identically zero; on return, KA[i] contains the fre-
  quency of X in the ith subinterval;
begin integer i, L; real BAK, XP;
  BAK := (B−A)/K;
  for i := 1 step 1 until N do begin
    XP := (X[i]−A)/BAK;
    L := entier (XP);
    if XP = L then go to p2 else L := L + 1; go to p5;
p2: if IUL = 0 then go to p3 else if L = 0 then L := L + 1;
      go to p5;
p3: if XP ≠ K then L := L + 1;
p5: KA[L] := KA[L] + 1;
  end;
end FREQUENCY
```

ALGORITHM 213
FRESNEL INTEGRALS

MALCOLM D. GRAY
The Boeing Co., Seattle, Wash.

real procedure *FRESNEL* (*w*, *S*, *C*); **value** *w*; **real** *S*, *C*;
comment *FRESNEL* computes the Fresnel sine and cosine integrals $S(w) = \int_0^w \sin[(\pi/2)t^2]\,dt$ and $C(w) = \int_0^w \cos[(\pi/2)t^2]\,dt$ using the series expansions

$$S(w) = w\sum_{i=1}^{\infty} \frac{(-1)^{i+1}x^{2i-1}}{(4i-1)(2i-1)!} \quad \text{and}$$

$$C(w) = w\sum_{i=1}^{\infty} \frac{(-1)^{i+1}x^{2i-2}}{(4i-3)(2i-2)!}$$

for $|w| < \sqrt{22/\pi}$ and $x \equiv \pi w^2/2$, and using the asymptotic series

$$S(w) = \alpha - \frac{1}{\pi w}[P(x)\sin(x) + Q(x)\cos(x)],$$

$$C(w) = \alpha - \frac{1}{\pi w}[P(x)\cos(x) - Q(x)\sin(x)]$$

where $|w| \geqq \sqrt{22/\pi}$, $x \equiv \pi w^2/2$,

$$Q(x) = 1 - \sum_{i=2}^{\infty} \frac{(-1)^i(4i-5)!!}{(2x)^{2i-2}}, \quad P(x) = \sum_{i=1}^{\infty} \frac{(-i)^{i+1}(4i-3)!!}{(2x)^{2i-1}},$$

and $n!! \equiv n(n-2)(n-4)\cdots 1$. If $w \geqq 0$, then $\alpha = \frac{1}{2}$, or if $w < 0$, then $\alpha = -\frac{1}{2}$.

This algorithm is a translation of a FAP coded subroutine currently in use on the IBM 7094 at the Boeing Company. The FAP program yields the following errors when tested at 0.05 increments of x:

x	ΔS	ΔC
0.00, 1.00	$<1 \times 10^{-7}$	$<1 \times 10^{-7}$
1.05, 8.65	$<1 \times 10^{-6}$	$<1 \times 10^{-6}$
8.70, 10.30	3×10^{-6}	2×10^{-6}
10.35, 11.00	5×10^{-6}	4×10^{-6}
11.05, 12.15	$<1 \times 10^{-6}$	3×10^{-6}
12.20, 15.00	$<1 \times 10^{-6}$	$<1 \times 10^{-6}$

where ΔS and ΔC are the approximate average absolute deviations (over the range) from the reference. The user must supply $S(w) = C(w) = \pm\frac{1}{2}$ if $w \to \pm\infty$. REFERENCES: ALGORITHMS 88-90, J. L. Cundiff, *Comm. ACM*, May 1962; Born, M. and Wolf, E., *Principles of Optics*, Pergamon Press (1958), pp. 369-431;

```
begin real x, x2, eps, term; integer n; eps := 0.000001;
  x := w × w/0.6366198;
  x2 := -x × x; if x ≧ 11.0 then go to asympt;
  begin real frs, frsi;
        frs := x/3; n := 5; term := x × x2/6;
        frsi := frs + term/7;
loops: if abs(frs-frsi) ≦ eps then go to send; frs := frsi;
        term := term × x2/n/(n-1); frsi := frs + term/(n+n+1);
        n := n + 2; go to loops;
send:  S := frsi × w; end;
  begin real frc, frci;
        frc := 1; n := 4; term := x2/2; frci := 1 + term/5;
loopc: if abs(frc-frci) ≦ eps then go to cend; frc := frci;
        term := term × x2/n/(n-1); frci := frc + term/(n+n+1);
        n := n + 2; go to loopc;
cend:  C := frci × w; end; go to aend;
asympt: begin real S1, S2, half, temp; integer i;
        x2 := 4 × x2; term := 3/x2; S1 := 1 + term; n := 8;
        for i := 1 step 1 until 5 do begin n := n + 4;
          term := term × (n-7) × (n-5)/x2; S1 := S1 + term;
          if abs(term) ≦ eps then go to next; end i;
next:  for i := 1 step 1 until 5 do begin n := n + 4;
          term := term × (n-5) × (n-3)/x2; S2 := S2 + term;
          if abs(term) ≦ eps then go to final; end i;
final: if w < 0 then half := -0.5 else half := 0.5; term := cos(x);
  temp := sin(x); x2 := 3.1415927 × w;
  C := half + (temp×S1-term×S2)/x2;
  S := half - (term×S1+temp×S2)/x2;
  end;
aend:  end FRESNEL
```

CERTIFICATION OF ALGORITHM 213 [S20]
FRESNEL INTEGRALS [M.D. Gray, *Comm. ACM 6* (Oct. 1963), 617]

Malcolm Gray (Recd. 29 May 1964 and, revised, 11 June 1964)
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(now at The Boeing Company, Seattle, Wash.)

Necessary changes to the algorithm are:

(1) in the first line, replace
real *S*, *C*; with **real** *w*, *S*, *C*;
(2) in the formula for $P(x)$, replace $(-i)^{i+1}$ with $(-1)^{i+1}$
(3) the statement beginning
loopc: *if abs(frc-frci)*
should read
loopc: **if** *abs(frc-frci)*
(4) in the body, replace the line
next: **for** *i* := 1 **step** 1 **until** 5 **do begin** *n* := *n* + 4;
with the lines
next: *term* := *S2* := 0.5/*x*; *n* := 4;
for *i* := 1 **step** 1 **until** 5 **do begin** *n* := *n* + 4;

The procedure (with the above changes) was executed on the Burroughs B5000 at Stanford University and gave results as indicated in the algorithm.

Communications from Helmut Lotsch of the W. W. Hansen Laboratories, Stanford University, and from Harold Butler of the Los Alamos Scientific Laboratory, Los Alamos, New Mexico, state that they found these same errors, and after the corrections were made, similar results were obtained. Mr. Lotsch's work was done on the B5000 and Dr. Butler's work was done on the IBM 7090.

ALGORMITH 214
q-BESSEL FUNCTIONS $I_n(t)$

J. M. S. SIMÕES PEREIRA
Gulbenkian Scientific Computing Center, Lisbon, Portugal

```
procedure qBessel (t, q, n, j, s); integer n, j; real t, q, s;
  array s;
comment This procedure computes values of any q-Bessel function
  I_n(t) for n integer (positive, negative or zero) by the use
  of the well-known expansion
```

$$I_n(t) = \sum_{k=0}^{\infty} \frac{q^{\frac{1}{2}k(k-1)+\frac{1}{2}(n+k)(n+k-1)} t^{n+2k}}{(q)_k (q)_{n+k}}$$

```
  where |q| < 1, (q)_n = (1-q)(1-q^2) ··· (1-q^n), (q)_0 = 1 and
  1/(q)_{-n} = 0 (n=1, 2, 3, ···). (See L. Carlitz, The product of
  q-Bessel functions, Port. Math. 21 (1962), 5-9.) Moreover, j
  denotes the number of terms (at least 2) retained in the summation,
  and s[i] stands for the sum of the first i+1 terms of the
  expansion. This procedure has been translated into FORTRAN
  for the IBM 1620 and run successfully;
begin integer k, m, p; real c, u; m := abs(n); c := 1; if
  n = 0 then go to A;
for p := 1 step 1 until m do c := c × (1-q↑p); if n < 0 then
  go to B;
A: u := q ↑ (n×(n-1)/2) × (t↑n)/c; s[0] := u;
for k = 1 step 1 until j do
begin u := u × q ↑ (n+2×k-2) × (t↑2)/((1-q↑k)×(1-q↑(n+k)));
  s[k] := s[k-1] + u end;
B: u := q↑((m-1)×m/2) × t ↑ (n+2×m)/c; s[m] := u;
for k := m + 1 step 1 until j do
begin u := u × q ↑ (n+2×k-2) × (t↑2)/((1-q↑k)(1-q↑(n+k)));
  s[k] := s[k-1] + u end
end
```

REMARK ON ALGORITHM 214
q-BESSEL FUNCTIONS $I_n(t)$ [J. M. S. Simões Pereira, *Comm. ACM 6* (Nov. 1963), 662]

J. M. S. SIMÕES PEREIRA (Recd 6 Jan 1964)
Gulbenkian Scientific Computing Center, Lisbon, Portugal

Corrections:

1. Insert a dummy statement labeled *C* just before the final **end**.
2. Add a statement **go to** *C* just before the label *B*.
3. Add a colon in the clause **for** *k* := 1 **step** 1 **until** *j* **do** ...

ALGORITHM 215
SHANKS

HENRY C. THACHER, JR.*
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* Work supported by the U. S. Atomic Energy Commission

```
procedure Shanks (nmin, nmax, kmax, S);
value nmin, nmax, kmax;
integer nmin, nmax, kmax;
array S;
comment This procedure replaces the elements S[nmin] through
  S[nmax−2×kmax] of the array S by the e[kmax] transform of
  the sequence S. The elements S[nmax−2×kmax+1] through
  S[nmax−1] are destroyed. The e[k] transforms were discovered
  by D. Shanks (J. Math. Phys. 34 (1955), 1–42). e[1] is equivalent
  to the (delta) ↑ 2 transformation. The e[k] transforms are par-
  ticularly valuable in estimating B in sequences which may be
  written in the form S[n] = B + ∑ a[i] × q[i] ↑ n  (i=1, 2, ··· ,
  k).
    The transformation is carried out by the epsilon algorithm
  (Wynn, P., M.T.A.C 10 (1956), 91–96). ALGOL procedures for
  applying the algorithm to series of complex terms are given by
  Wynn (BIT 2 (1962), 232–255).
    The body of this procedure has been tested using the Dart-
  mouth Self-Contained ALGOL Processor for the LGP-30 com-
  puter. It gave the following results on the sequence for the
  smaller zero of the Laguerre polynomial, L[2](x):

    n      S[n]        e[1](S[n])      e[2](S[n])      e[1]²(S[n])
    0   0.0000000   0.5714285   0.5857432   0.5857616
    1   0.5000000   0.5851059   0.5857854   0.5857859
    2   0.5625000   0.5857318   0.5857861   0.5857861
    3   0.5791016   0.5857816
    4   0.5838396   0.5857859
    5   0.5852172
    6   0.5856198        True Value  0.5857864375

  These results are in satisfactory agreement with those given by
  by Wynn (1956);
begin integer j, k, limj, limk, two kmax;
  real T0, T1;
  two kmax := kmax + kmax;
  limj := nmax;
for j := nmin step 1 until limj do
  begin T0 := 0;
  lim := j − nmin;
  if limk > two kmax then limk := two kmax⟩  limk := limk − 1;
  for k := 0 step 1 until limk do
    begin T1 := S [j−k] − S [j−k−1];
      if T1 ≠ 0 then T1 := T0 + 1/T1 else
      if S [j−k] = 1099 then T1 := T0 else
        T1 := 1099;
      comment 1099 may be replaced by the largest number
        representable in the computer;
      T0 := S [j−k−1];
      S [j−k−1] := T1
    end for k
  end for j
end Shanks
```

CERTIFICATION OF ALGORITHM 215
SHANKS [H. C. Thacher, Jr., *Comm. ACM 6* (Nov. 1963), 662]

LARRY SCHUMAKER (Recd. 16 Dec. 63)
Computation Ctr., Stanford U., Stanford, Calif.

Algorithm 215 was coded in Extended ALGOL for the Burroughs B-5000 and was tested on a large number of sequences. One apparent typographical error was noted. The statement *lim* := *j* − *nmin* should have read *limk* := *j* − *nmin*. The following tables were reproduced exactly: (a) tables on p. 5 and p. 33 of [1]; (b) Table I on p. 95 of [2]; (c) Tables III and IV on p. 28 of [3].

REFERENCES:

1. SHANKS, D. Non-linear transformations of divergent and slowly convergent sequences. *J. Math. Phys. 34* (1955), 1–42.
2. WYNN, P. On a device for computing the $e_m(S_n)$ transformation. *MTAC 10* (1956), 91–96.
3. WYNN, P. On repeated application of the ϵ-algorithm. *Chiffres 4* (1961), 19–22.

ALGORITHM 216
SMOOTH
RICHARD GEORGE*
Argonne National Laboratory, Argonne, Ill.
* Work supported by the U. S. Atomic Engergy Commission.

```
procedure SMOOTH (Data) which is a list of length: (n);
  integer n; real array Data;
  begin
    comment This procedure accomplishes fourth-order smooth-
      ing of a list using the method given by Lanczos, Applied
      Analysis (Prentice-Hall, 1956). This algorithm requires only
      one additional list for temporary storage;
    real Factor, Top; integer Max I, I, J; array Delta [1 : n];
    Factor := 3.0/35.0;
    Max I := n - 1;
    for I := 1 step 1 until Max I do
      Delta [I] := Data [I+1] - Data [I];
    for J := 1 step 1 until 3 do
      begin
        Top := Delta [1];
        Max I := Max I - 1;
        for I := 1 step 1 until Max I do
          Delta [I] := Delta [I+1] - Delta [I]
      end;
    Max I := n - 2;
    for I := 3 step 1 until Max I do
      Data [I] := Data [I] - Delta [I-2] × Factor;
    Data [1] := Data [1] + Top/5.0 + Delta [1] × Factor;
    Data [2] := Data [2] - Top × 0.4 - Delta [1]/7.0;
    Data [n] := Data [n] - Delta [n-3]/5.0 + Delta [n-4] × Factor;
    Data [n-1] := Data [n-1] + Delta [n-3] × 0.4 - Delta
      [n-4]/7.0
  end;
```

ALGORITHM 217
MINIMUM EXCESS COST CURVE
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Marathon Oil Co., Findlay, Ohio

```
procedure MINIMUM EXCESS COST CURVE (nodes, links,
  source, sink, I, J, crash, normal, slope, node, lij, ERROR);
value nodes, links, source, sink;
integer nodes, links, source, sink;
integer array I, J, crash, normal, slope, node, lij;
comment This procedure utilizes a network-type description of
  a project to compute the minimum cost involved in expedition
  of the project completion date. Project tasks are identified and
  completion order specified by the vector pair I, J, which contain
  node numbers of the events starting and ending each task. The
  tasks are parameterized within the vectors crash, normal, and
  slope—which contain the crash or minimum task completion
  times, the normal task completion times, and the increased cost
  per unit decrease in task duration (the slope of the time-cost
  curve), which must be a nonzero integer. The procedure initially
  determines the normal-duration critical path, then successively
  reduces the durations of the tasks with the flattest cost slope,
  adjusting the critical path, until minimum durations are
  reached. The FORD-FULKERSON labeling technique is
  utilized. Each task must proceed from a lower-numbered node
  to a higher-numbered one—if not, exit to the nonlocal label
  ERROR is made. Nodes should be numbered sequentially, start-
  ing at the initial event (source) and continuing to the final event
  (sink). The maximum node number is equivalent to the value
  nodes, while the value links denotes the total number of tasks.
  The arrays are of dimensions I, J, crash, normal, slope,
  lij [1:links] and node [1:nodes];
begin integer m, n, tb, nji, nij, lex, kf, nj, ni, ntv, ord, infinity,
    temp;
  integer array labl[1:nodes,1:3], f[1:links,1:2];
  comment infinity is herein used to represent the largest avail-
    able integer;
  for m := 1 step 1 until links-1 do
    if I[m] ≧ J[m] ∨ I[m] > I[m+1] ∨ J[m] > J[m+1] then go
      to ERROR;
  if I[links] ≧ J[links] then go to ERROR;
  for n := 1 step 1 until nodes do labl[n, 1] := labl[n, 2] :=
    labl[n, 3] := node[n] := 0;
  for m := 1 step 1 until links do
    begin f[m, 1] := f[m, 2] := 0;
      temp := node[I[m]] + normal[m];
      if node [J[m]] < temp then node [J[m]] := temp
    end;
  ntv := ord := 0;  tb := node[sink];
A:  labl[source, 1] := source;  labl[source, 3] := infinity;
    for m := 1 step 1 until links do
      begin if labl[I[m], 1] = 0 then go to B;
        if labl[J[m], 1] ≠ 0 then go to C;
        nji := node[J[m]] − node[I[m]];
        if nji ≠ normal[m] then go to A1;
        lex := slope[m] − f[m, 1];
        if lex ≦ 0 then go to A1;
        kf := 1;  go to A2;
A1: if nji ≠ crash[m] then go to C;
    lex := infinity;  kf := 2;
A2: labl[J[m], 1] := I[m];  labl[J[m], 2] := kf;
    if labl[I[m], 3] > lex then go to A3;
    labl[J[m], 3] := labl[I[m], 3];  go to A4;
A3: labl[J[m], 2] := lex;
A4: if J[m] = sink then go to D else go to C;
B:  if labl[J[m], 1] = 0 then go to C;
    nij := node[I[m]] − node[J[m]];
    if nij ≠ normal[m] ∨ f[m, 1] = 0 then go to B1;
    lex := f[m, 1];  kf := −1;  go to B2;
B1: if nij ≠ normal[m] ∨ [m, 2] = 0 then go to C;
    lex := f[m, 2];  kf := −2;
B2: labl[I[m], 1] := J[m];  labl[I[m], 2] := kf;
    if [labl[J[m], 3] > lex then go to B3;
    labl[I[m], 3] := labl[J[m], 3];  go to B4;
B3: labl[I[m], 3] := lex;
B4: if I[m] = sink then go to D;
C:  end;
    for n := 1 step 1 until nodes do if labl[n, 1] = 0 then
      node[n] := node[n] − 1;
F:  for n := 1 step 1 until nodes do labl[n, 1] := labl[n, 2] :=
      labl[n, 3] := 0;
    go to A;
D:  if labl[sink, 3] = infinity then go to OUT;
    ntv := ntv + labl[sink, 3];  nj := sink;
G:  ni := labl[nj, 1];
    if labl[nj, 2] > 0 then go to G1;
    for m := 1 step 1 until links do if I[m] = nj ∧ J[m] =
      ni then f[m, −labl[nj, 2]] := f[m, −labl[nj, 2]] +
      labl[sink, 3];
G1: for m := 1 step 1 until links do if I[m] = ni ∧ J[m] =
      nj then f[m, labl[nj, 2]] := f[m, labl[nj, 2]] + labl[sink, 3];
    if ni = source then go to OUT;
    nj := ni;  go to G;
OUT: for m := 1 step 1 until links do
      begin lij[m] := node[J[m]] − node[I[m]];
        if lij[m] > normal[m] then lij[m] := normal[m]
      end;
    ord := (tb-node[sink]) × ntv;  tb := node[sink];
    if labl[sink, 3] = infinity then ntv := infinity;
ANS: comment as control passes through here—
      ord is the ordinate of the minimum project excess cost
        curve at a total project duration of node[sink],
      successive values of ord plotted versus node[sink] gener-
        ate the minimum project excess cost curve.
      node[1:nodes] contains the event times at each node
      lij[1:links] contains the durations of each task
      ntv is the slope of the cost curve back in time from total
        duration node[sink].
      these values should be printed in some readable form;
    if ntv < infinity then go to F;
end MINIMUM EXCESS COST CURVE;
```

REMARK ON ALGORITHM 217 [H]
MINIMUM EXCESS COST CURVE [William A. Briggs, *Comm. ACM 6* (Dec. 1963), 737]

JOHN F. MUTH. (Recd. 26 Dec. 1967)
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KEY WORDS AND PHRASES: critical path scheduling, PERT, cost/time tradeoffs, network flows

CR CATEGORIES: 3.59, 5.41.

Algorithm 217 was transliterated into FORTRAN and successfully run on the CDC 3600 system at Indiana University after the following changes were made:

(1) In the first Boolean expression of the program the term:
$J[m] \geq J[m+1]$
was replaced by the term:
$(I[m] = I[m+1] \wedge J[m] \geq J[m+1])$

(2) The line:
*A*3: *labl*[*J*[*m*], 2] := *lex*;
was replaced by:
*A*3: *labl*[*J*[*m*], 3] := *lex*;

(3) In the statement labeled *B*1, the symbols:
[*m*,2] = 0
were replaced by:
f[*m*, 2] = 0

(4) Two statements before the statement labeled A was replaced by
*ntv*1 := *ntv* := *ord* := 0
where *ntv*1 was an additional integer variable. The third statement before *ANS* was replaced by:
ord := (*tb-node*[*sink*]) × *ntv*1 + *ord*; *ntv*1 := *ntv*;

ALGORITHM 218
KUTTA MERSON

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```
procedure KuttaMerson (n, t, y, eps, h, fct, first);
value n, eps;
integer n;
real t, eps, h;
real array y;
Boolean first;
```

* Work supported by the U. S. Atomic Energy Commission.

```
procedure fct;
comment This procedure integrates the system of ordinary first-
  order differential equations y[i] = f[i](t, y[1], y[2], ··· y[n]) from
  t = t to t = t + h by the Kutta-Merson method (L. Fox, Numeri-
  cal Solution of Ordinary and Partial Differential Equations,
  p. 24, Pergamon Press, 1962). The working interval of calcula-
  tion is adjusted by the procedure so that the maximum absolute
  error of the dependent variables is less than eps. For optimum
  error control, the equations should be scaled so that all de-
  pendent variables have approximately the same magnitude.
  Input variables for the procedure are n, the number of equa-
  tions, t, initial value of the independent variable, y, array of
  initial values of dependent variables, eps, allowable error, h,
  the total interval, fct, a procedure evaluating the derivatives,
  and first, a Boolean variable which indicates whether the work-
  ing interval has been adjusted to secure the desired accuracy.
  On the initial call of the procedure for a given system, first
  should be true. It will be set false by the procedure, and the
  proper working interval determined. The procedure fct has as
  formal parameters the simple real variable t, and the real
  arrays y and f. For i = 1, 2, 3, ··· , n it must assign to f[i] the
  value of the first derivative of y[i] appropriate to the values of t
  and y. The body of this procedure has been tested using the
  Dartmouth SCALP compiler for the LGP-30 computer. For the
  equation dy/dt = -2ty² and input data t = 1, y = .5, h = 1,
  eps = .0001, the average error was .000003 and the time was 30
  min. For the linear boundary value problem d²y/dt² = -1 -
  (t²+1)y, y(±1) = 0, the maximum error was .0000024 (L.
  Collatz, The Numerical Treatment of Differential Equations, pp.
  145, 225, Springer-Verlag, Berlin, 1960) and the time, 90 min.
  More accuracy may be achieved by using a smaller value of eps;
begin integer i, loc;
  real error;
  array y0, y1, y2, f0, f1, f2[1:n];
  own integer ploc;
  own real hc;
  Boolean increase;
  if first then begin hc := h; ploc := 1; first := false end;
  loc := 0;
next: fct(t, y0, f0);
  for i := 1 step 1 until n do
  y1[i] := y0[i] + hc/3 × f0[i];
  fct(t + hc/3, y1, f1);
  for i := 1 step 1 until n do
  y1[i] := y0[i] + hc/6 × f0[i] + hc/6 × f1[i];
  fct(t + hc/3, y1, f1);
  for i := 1 step 1 until n do
  y1[i] := y0[i] + hc/8 × f0[i] + 3 × hc/8 × f1[i];
  fct(t + hc/2, y1, f2);
  for i := 1 step 1 until n do
  y1[i] := y0[i] + hc/2 × f0[i] - 3 × hc/2 × f1[i] + 2 × hc ×
    f2[i];
  fct(t + hc, y1, f1);
  for i := 1 step 1 until n do
  y2[i] := y0[i] + hc/6 × f0[i] + 2 × hc/3 × f2[i] + hc/6 × f1[i];
  increase := true;
  for i := 1 step 1 until n do
  begin error := abs(.2 × (y1[i] - y2[i]));
    comment To test on relative error change this expression to
      abs(.2 - .2 × y2[i]/y1[i]);
    if error > eps then
    begin hc := hc/2;
      ploc := 2 × ploc;
      loc := 2 × loc;
      go to next
    end;
    if error × 64 > eps then increase := false
  end i;
  t := t + hc;
  for i := 1 step 1 until n do
  y0[i] := y2[i];
  loc := loc + 1;
  if loc < ploc ∧ increase ∧ loc = loc ÷ 2 × 2 ∧ ploc > 1 then
  begin hc := 2 × hc;
    loc := loc ÷ 2;
    ploc := ploc ÷ 2
  end;
go to next
end KuttaMerson
```

CERTIFICATION OF ALGORITHM 218 [D2]
KUTTA MERSON [Phyllis M. Lukehart, *Comm. ACM* 6 (Dec. 1963), 737]

KAREN BORMAN PRIEBE (Recd. 10 Feb. 1964)
Woodward Governor Company, Rockford, Illinois

Algorithm 218 was translated into FAST for the NCR 315 and gave satisfactory results with the following corrections, if the equations were scaled as recommended in the comment of the original algorithm. Ignoring this scaling can lead to results that do not satisfy the intended error criterion.

1. **procedure** *KuttaMerson (n, t, y, eps, h, fct, first, x);*
instead of
procedure *KuttaMerson (n, t, y, eps, h, fct, first);*
2. **real array** *y, x;*
instead of
real array *y;*
3. **if** *first* **then begin for** *i* := 1 **step** 1 **until** *n* **do** *y0[i]* := *y[i]*;
hc := *h*;
instead of
if *first* **then begin** *hc* := *h*; ···

```
4.    if loc < ploc then
      begin
        if increase ∧ loc = (loc÷2) × 2 ∧ ploc > 1 then
        begin
          hc := 2 × hc;
          loc := loc ÷ 2;
          ploc := ploc ÷ 2
        end;
        go to next
      end;
      for i := 1 step 1 until n do x[i] := y0[i];
    end KuttaMerson
```

instead of

```
      if loc < ploc ∧ increase ···
    end KuttaMerson
```

5. The following sentences should be added to the initial comment of the procedure:

The values of the dependent variables at $t + h$ are placed in the array x. Note that the values of t and *first* are changed as side-effects of the procedure. {As originally written, *KuttaMerson* seemed unable to obtain the values of the solution at t or to transmit the values of the solution at $t + h$ to the outside program!—Ed.}

6. Change *array* to **array** in the body of the procedure.

7. Insert after **own integer** *ploc*;

```
own array y0[1:n];
```

Delete *y*0 from the existing array declaration.

REMARK ON ALGORITHM 218 [D2]
KUTTA-MERSON [Phyllis M. Lukehart, *Comm. ACM 6* (Dec. 1963), 737]

G. BAYER (Recd. 25 Oct. 1965)
Technische Hochschule, Braunschweig, Germany

Successive calls of *Kutta Merson* with *first* ≡ **false** do not reach the upper bound $t+h$ if the interval h is unequal to the interval h of the first call with *first* ≡ **true**.

Proposed correction:

1) declaration **real** *hc*, instead of **own real** *hc*;
2) **if** *first* **then begin for** *i* := 1 **step** 1 **until** *n* **do** *y*0[*i*] := *y*[*i*];
   hc := *h*; *ploc* := 1; *first* := **false**
   end else *hc* := *h*/*ploc*;
   instead of **if** *first* **then begin** ··· **end**;

ALGORITHM 219

TOPOLOGICAL ORDERING FOR PERT NETWORKS

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```
procedure Topological Ordering (i, j, tri, n, ne);
integer n, ne; integer array i, j, tri;
comment Nodal points i and j represent activities in a PERT
  network. n is the number of activities. tri is a tape record index
  vector locating where additional data for each activity is stored.;
begin integer a, b; integer array ni, nj, event [1:n];
  comment An event vector is set up containing ne events.
    New nodal numbers ni and nj are assigned for all activities.;
  ne := ni[1] := 1; event[1] := i[1];
  begin for a := 2 step 1 until n do
    begin for b := 1 step 1 until ne do
    if i[a] = event[b] then begin ni[a] := b;
    go to repeat 1 end;
    end;
  ni[a] := ne := ne + 1; event[ne] := i[a];
repeat 1: end;
  begin for a := 1 step 1 until n do
    begin for b := 1 step 1 until ne do
    if j[a] = event[b] then begin nj[a] := b;
    go to repeat 2 end;
    end;
  nj := ne := ne + 1; event[ne] := j[a];
repeat 2: end;
  begin integer t, bigtal; integer array rank, con[1:ne];
  comment Event ranking (topological ordering);
  for a := 1 step 1 until ne do
    begin rank[a] := 1; con[a] := 0 end;
    bigtal := 1;
  pass: t := 0;
    for a := 1 step 1 until n do
      begin if rank[nj[a]] ≦ rank[ni[a]] then
      rank[nj[a]] := rank[ni[a]] + 1 else go to fill;
      if rank[nj[a]] > bigtal then
      bigtal := rank[nj[a]]; t := 1
  fill: con[rank[ni[a]]] := con[rank[nj[a]]] := 1
      end;
    if t ≦ 0 then go to new;
    for a := 1 step 1 until bigtal do
      begin if con[a] = 0 then go to Loop end;
      comment Loop should be a label of a procedure statement
        which calls a subroutine to detect those events which may
        be in a loop in the PERT network or the label of a print out
        indicating that loop(s) exist in the network. In any case
        a loop exists and further problem processing is impossible.;
    for a := 1 step 1 until bigtal do con[a] := 0;
    go to pass;
    comment Reassignment of a new nodal number, ni, to all
      activities;
  new: t := 1:
   for a := 1 step 1 until bigtal do
     begin for b := 1 step 1 until ne do
     if rank[b] = a then begin event[b] := t; t := t +1 end
     end;
   for a := 1 step 1 until n do ni[a] := event[ni[a]]
   end;
   comment Using the new nodal number, ni, activities (i and j)
     and their corresponding tri may now be arranged in topological
     sequence with conventional sort routines. Sorting should be
     done on ni.;
end
```

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REMARK ON ALGORITHM 219

Topological Ordering for PERT Networks

[R. H. Kase, *Comm. ACM 6*, 12 (Dec. 1963), 738–739]
Dennis Tenney [Rec 31 Jan. 1977 and 14 March 1976]
Knutson and Associates, 1700 North 55th St., Boulder, CO 80301.

ACM Algorithm 219 has been implemented successfully with two necessary modifications:

(1) change

```
  end;
  ni[a] := ne := ne +1; event[ne] := i[a];
  repeat 1: end;
```

to

```
  ni[a] := ne := ne+1; event[ne] := i[a];
  repeat 1: end;
  end;
```

(2) change

```
  end;
  nj := ne := ne+1; event[ne] := j[a];
  repeat 2: end;
```

to

```
  nj[a] := ne := ne+1; event[ne] := j[a];
  repeat 2: end;
  end;
```

ALGORITHM 220
GAUSS-SEIDEL

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```
procedure GAUSS-SEIDEL (n, A, B, tol);
  value n, tol; array A, B; real tol; integer n;
comment GAUSS-SEIDEL solves a system, Ax = B, of n
  simultaneous linear equations in n unknowns. A is the matrix of
  coefficients, B an inhomogeneous vector. The standard Gauss-
  Seidel iterative technique is employed until | x_K^(i) - x_K^(i-1) | < tol
  for all K, where x_K^(i) denotes the ith iterant of the unknown x_K .
  (Cf. Ralph G. Stanton, Numerical Methods for Science and Engi-
  neering, Ch. 8);
begin array X, Y[1:n]; integer i, j, K;
  for i := 1 step 1 until n do X[i] := Y[i] := 0;
START: for i := 1 step 1 until n do
          begin Y[i] := B[i];
            for j := 1 step 1 until n do
            Y[i] := if i = j then y[i] else
              Y[i] - A[i, j] × Y[j];
            Y[i] := Y[i]/A[i, i]
          end i;
comment Now test for convergence;
  for K := 1 step 1 until n do
    if abs(Y[K] - X[K]) ≥ tol then
    begin for i := 1 step 1 until n do
      X[i] := Y[i]; go to START
    end convergence test;
end GAUSS-SEIDEL
```

CERTIFICATION OF AND REMARK ON ALGORITHM 220
GAUSS-SEIDEL [P. W. Shantz, *Comm. ACM 6* (Dec. 1963), 739]

A. P. BATSON (Recd 6 Jan. 1964)
University of Virginia, Charlottesville, Va.
NIKLAUS WIRTH (Recd 6 Jan. 1964)
Computer Science Div., Stanford U., Stanford, Calif.

[EDITOR'S NOTE. Two substantially equivalent contributions were received on the same day, and so the editor has merged them.—G.E.F.]

The following errors were detected.

1. The procedure cannot communicate the solution to the outside block unless X (or Y) is made a parameter of the procedure.
2. The identifier *GAUSS-SEIDEL* may not contain a hyphen.
3. In the fourth line after the label *START* change $y[i]$ to $Y[i]$.

With the above errors corrected, *GAUSS SEIDEL* was successfully run on the Stanford 7090 computer in Wirth's Extended ALGOL, and on the Virginia ALGOL compiler for the Burroughs 205.

The following improvements would be desirable.

1. Avoid repeated reference to the subscripted variable $Y[i]$ inside the j loop.
2. Permit the user to initialize the array X to an appropriate value at the start of the iteration.
3. Modify *tol* to be a relative error, rather than an absolute error.
4. Incorporate a guard against nonconvergence.