

ALGORITHM 361  
 PERMANENT FUNCTION OF A SQUARE  
 MATRIX I AND II [G6]

BRUCE SHRIVER, P. J. EBERLEIN, AND R. D. DIXON (Recd.  
 19 Feb. 1969, 7 Mar. 1969 and 9 July 1969)  
 State University of New York at Buffalo, Amherst, NY  
 14226

KEY WORDS AND PHRASES: matrix, permanent, determinant

CR CATEGORIES: 5.30

**real procedure** per1(*A*, *n*);  
**integer** *n*; **array** *A*;  
**comment** Let *A* be an  $n \times n$  real matrix,  $n > 1$ . The permanent function of *A*, denoted per(*A*), is computed by H. J. Ryser's [1] expansion formula:

$$\text{per}(A) = \sum_{r=0}^{n-1} (-1)^r \sum_{x \in T_{n-r}} \prod_{i=1}^r x_i$$

where  $T_j$ ,  $j = n, n-1, \dots, 2, 1$ , is the set of vectors  $x = (x_i)$ ,  $i = 1, 2, \dots, n$  which are obtained by adding  $j$  columns of *A* together in all  $\binom{n}{j}$  possible ways. To effect the sum over vectors in  $T_j$ ,  $n-1$  sums are computed. The natural 1-1 map from the binary integers to all  $r$ -combinations,  $r = 1, 2, \dots, n-1$ , is used to increment the sums over the sets  $T_j$ .

REFERENCE:

1. RYSER, H. J. *Combinatorial Mathematics, Carus Monograph* #14. Wiley, New York, 1963, p. 27;

**begin**  
**real** *sig*, *pera*, *prod*, *rowsum*;  
**integer** *number*, *limit*, *mod*, *gen*, *g*, *i*, *j*, *r*;  
**array** *sum*[0:*n*-1];  
**integer array** *d*[1:*n*];  
*sig* := -1; *pera* := 0; *limit* :=  $(2 \uparrow n) - 1$ ;  
**for** *r* := 0 **step** 1 **until** *n* - 1 **do** *sum*[*r*] := 0;  
**for** *number* := 1 **step** 1 **until** *limit* **do**  
**begin**  
*r* := 0; *gen* := *number*;  
**for** *mod* := 1 **step** 1 **until** *n* **do**  
**begin**  
*g* := *gen* ÷ 2; **if** (*gen* - *g* × 2) = 1 **then**  
**begin** *r* := *r* + 1; *d*[*r*] := *mod* **end**;  
*gen* := *g*  
**end**;  
*prod* := 1;  
**for** *i* := 1 **step** 1 **until** *n* **do**  
**begin**  
*rowsum* := 0;  
**for** *j* := 1 **step** 1 **until** *r* **do**  
*rowsum* := *rowsum* + *A*[*i*, *d*[*j*]];  
*prod* := *prod* × *rowsum*  
**end**;  
*sum*[*n* - *r*] := *sum*[*n* - *r*] + *prod*  
**end**;  
**for** *r* := 0 **step** 1 **until** *n* - 1 **do**  
**begin** *sig* := -*sig*; *pera* := *pera* + *sig* × *sum*[*r*] **end**;  
*per* := *pera*  
**end** of real procedure per1;

**real procedure** per2(*A*, *n*);  
**integer** *n*; **array** *A*;  
**comment** Let *A* be an  $n \times n$  real matrix,  $n > 1$ . The permanent function of *A*, denoted by per(*A*) is computed by Jurkat and Ryser's [1] method of inductively generating the vectors  $p_1, \dots, p_n$  where  $p_r$  is the vector of permanents of  $r$  by  $r$  submatrices of the first  $r$  rows of *A*. This vector has  $\binom{n}{r}$  components

indexed by the  $r$ -combinations of  $\{1, \dots, n\}$ . The natural 1-1 map from the binary integers  $\{1, \dots, 2 \uparrow n - 1\}$  to the  $r$ -combinations of  $\{1, \dots, n\}$  for  $r = 1, \dots, n$  is used to index the  $p$ 's and thus they are generated in an order somewhat different from that of Jurkat and Ryser.

REFERENCE:

1. JURKAT, W. B. AND RYSER, H. J. Matrix factorizations of determinants and permanents. *J. Algebra* 3 (1966), 1-27;

**begin**  
**integer** *number*, *limit*, *mod*, *gen*, *g*, *r*, *dig*, *sub*, *j*;  
**array** *list* [1:2  $\uparrow$  *n*-1];  
*limit* := 2  $\uparrow$  *n* - 1;  
**comment** Initialize list as accumulators;  
**for** *j* := 1 **step** 1 **until** *limit* **do** *list* [*j*] := 0;  
**for** *j* := 1 **step** 1 **until** *n* **do** *list* [2  $\uparrow$  (*j*-1)] := *A*[1, *j*];  
**for** *number* := 1 **step** 1 **until** *limit* **do**  
**begin**  
**if** *list* [*number*]  $\neq$  0 **then**  
**begin**  
*r* := 1; *gen* := *number*;  
**for** *mod* := 1 **step** 1 **until** *n* **do**  
**begin**  
*g* := *gen* ÷ 2;  
**if** *gen* - 2 × *g* = 1 **then** *r* := *r* + 1;  
*gen* := *g*  
**end** count of 1's in *number*;  
*dig* := 1; *gen* := *number*;  
**for** *mod* := 1 **step** 1 **until** *n* **do**  
**begin**  
*g* := *gen* ÷ 2;  
**if** *gen* - 2 × *g* = 0 **then**  
**begin**  
*sub* := *number* + *dig*;  
*list* [*sub*] := *list* [*sub*] + *list* [*number*] × *A* [*r*, *mod*]  
**end**;  
*gen* := *g*; *dig* := 2 × *dig*  
**end** computations with *list* [*number*];  
**end**  
**end**;  
*per* := *list* [*limit*]  
**end** of real procedure per2;

Note. On the Permanent Function of a Square Matrix I and II: Program I is slower than Program II. However Program II uses approximately  $2^n$  more locations of store. The running times for both programs double when  $n$  is incremented by 1.

ALGORITHM 362  
 GENERATION OF RANDOM PERMUTATIONS [G6]

J. M. ROBSON (Recd. 1 Apr. 1969)  
 Programming Research Group, 45 Banbury Road, Oxford,  
 England

KEY WORDS AND PHRASES: permutation, random permutation, transposition

CR CATEGORIES: 5.5

**procedure** perm(*n*, *r*, *A*); **value** *n*, *r*; **integer** *n*, *r*; **integer**  
**array** *A*;

**comment** This procedure produces in the vector *A* a permutation on the integers 1, 2,  $\dots$ ,  $n$ , each of the  $n!$  permutations being given by one value of  $r$  between 1 and  $n!$  inclusive. It is thus similar in effect to the procedure given in [1] but it is considerably faster, especially for large values of  $n$ , since it uses a single loop rather than a double one.

A permutation is generated as the product of  $n-1$  transpositions of which the  $j$ th transposes  $A[n+1-j]$  and  $A[x]$  for some  $x \leq n+1-j$ .

If the line  
**for**  $i := 1$  **step** 1 **until**  $n$  **do**  $A[i] := i$   
 is omitted the procedure will permute the original values  
 $A[1], \dots, A[n]$  in the same manner.

REFERENCE:

1. ROBINSON, C. L. Algorithm 317, Permutation. *Comm. ACM* 10 (Nov. 1967), 729;

```

begin
  integer  $i, x, y$ ;
  for  $i := 1$  step 1 until  $n$  do  $A[i] := i$ ;
  for  $i := n$  step -1 until 2 do
    begin
       $x := r - (r \div i) \times i + 1$ ;  $r := r \div i$ ;
       $y := A[x]$ ;  $A[x] := A[i]$ ;  $A[i] := y$ 
    end
  end

```

### ALGORITHM 363 COMPLEX ERROR FUNCTION\* [S15]

WALTER GAUTSCHI (Recd. 11 June 1969)  
 Computer Sciences Department, Purdue University, La-  
 fayette, IN 47907

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 Space Administration (NASA) under grant NGR 15-005-039  
 and, in part, by Argonne National Laboratory.

KEY WORDS AND PHRASES: error function for complex  
 argument, Voigt function, Laplace continued fraction, Gauss-  
 Hermite quadrature, recursive computation

CR CATEGORIES: 5.12

```

procedure  $wofz(x, y, re, im)$ ; value  $x, y$ ; real  $x, y, re, im$ ;
comment This procedure evaluates the real and imaginary
  part of the function  $w(z) = \exp(-z^2)\text{erfc}(-iz)$  for arguments
   $z = x + iy$  in the first quadrant of the complex plane. The accu-
  racy is 10 decimal places after the decimal point, or better.
  For the underlying analysis, see W. Gautschi, "Efficient com-
  putation of the complex error function," to appear in SIAM
  J. Math. Anal.;

```

```

begin
  integer  $capn, nu, n, np1$ ;
  real  $h, h2, lambda, r1, r2, s, s1, s2, t1, t2, c$ ;
  Boolean  $b$ ;
  if  $y < 4.29 \wedge x < 5.33$  then
    begin
       $s := (1 - y/4.29) \times \text{sqrt}(1 - x \times x/28.41)$ ;
       $h := 1.6 \times s$ ;  $h2 := 2 \times h$ ;
       $capn := 6 + 23 \times s$ ;  $nu := 9 + 21 \times s$ 
    end
  else
    begin  $h := 0$ ;  $capn := 0$ ;  $nu := 8$  end;
    if  $h > 0$  then  $lambda := h2 \uparrow capn$ ;
     $b := h = 0 \vee lambda = 0$ ;
     $r1 := r2 := s1 := s2 := 0$ ;
    for  $n := nu$  step -1 until 0 do
      begin
         $np1 := n + 1$ ;
         $t1 := y + h + np1 \times r1$ ;  $t2 := x - np1 \times r2$ ;
         $c := .5/(t1 \times t1 + t2 \times t2)$ ;
         $r1 := c \times t1$ ;  $r2 := c \times t2$ ;
        if  $h > 0 \wedge n \leq capn$  then
          begin
             $t1 := lambda + s1$ ;  $s1 := r1 \times t1 - r2 \times s2$ ;
             $s2 := r2 \times t1 + r1 \times s2$ ;
             $lambda := lambda/h2$ 
          end
        end
      end

```

```

end;
 $re := \text{if } y = 0 \text{ then } \exp(-x \times x) \text{ else}$ 
   $1.12837916709551 \times (\text{if } b \text{ then } r1 \text{ else } s1)$ ;
 $im := 1.12837916709551 \times (\text{if } b \text{ then } r2 \text{ else } s2)$ 
end wofz

```

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)

The Plessey Co. Ltd., Roke Manor, Romsey, Hants,  
 England

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 com-  
 puter.

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 prece-  
 dence 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 state-  
 ment 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  $p := \text{Gamma}$   
 $[m+n+1]$  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 begin-  
 ning **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 begin-  
 ning

```

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**;

$k := n - i$ ;

$p := p + \text{Gamma}[2 \times k + 3] \times z / \text{Gamma}[i] \times \text{Gamma}[k + 2] \times \text{Gamma}[k - i - m + 3]$ ;

$z := z \times y$

**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.

## CERTIFICATION OF ALGORITHM 255 [C6] COMPUTATION OF FOURIER COEFFICIENTS

[Linda Teijelo, *Comm. ACM* 8 (May 1965), 279]

GILLIAN HALL\* AND VALERIE A. RAY† (Recd. 31 Mar. 1969 and 1 July 1969)

National Physical Laboratory, Teddington, Middlesex, England

\* M.R.C. team, Division of Computer Science (formerly of Division of Numerical and Applied Mathematics).

† Division of Numerical and Applied Mathematics.

KEY WORDS AND PHRASES: numerical integration, Fourier coefficients, Filon's method

CR CATEGORIES: 5.16

The algorithm was translated using the KDF9 Kidsgrove ALGOL compiler, and needed the following correction.

The tests for convergence on lines 51 and 83 should read respectively:

**if**  $\text{abs}(\text{prevint2} - \text{int2}) < \text{eps} \times \text{abs}(\text{int2}) \wedge n > 5$  **then**

**if**  $\text{abs}(\text{prevint1} - \text{int1}) < \text{eps} \times \text{abs}(\text{int1}) \wedge n > 5$  **then**

With this alteration, the program was tested successfully on a series of functions  $F(x)$  using a range of values of  $m$  and  $\text{eps}$  for each function. The parameter *subdivmax* was set at the recommended value, 10. For  $F(x) = x^2$ , for which the method is exact, results were obtained correct to machine accuracy, i.e.  $10\frac{1}{2}$  decimal places.

Remarks. (i) It would be better to declare the identifier *tn1* as type **integer**, i.e. to replace lines 20 and 21 of the text by:

$c0, c1, s0, s1, \text{int1}, \text{int2}, \text{prevint1}, \text{prevint2}, t3, \text{temp}$ ;

**integer**  $n, i, \text{tn1}$ ; **Boolean**  $\text{bool}$ ;

(ii) There is no indication, after execution of the algorithm, whether the computation was terminated because of apparent convergence or because the number of times,  $n$ , that the interval was halved became greater than *subdivmax*. The following modification provides such an indication; it has the effect that *cosine* and *sine* will retain their entry values except in the case where *cosine* or *sine* has the value *true* on entry and  $n$  becomes greater than *subdivmax* in the course of computation. In this case the value on exit will be *false*.

Line 3 becomes:

**value**  $\text{eps}, \text{subdivmax}, m$ ; **real**  $\text{eps}, \text{cint}, \text{sint}$ ;

Line 57 becomes:

$\text{sint} := \text{int2}$ ;  $\text{sine} := \text{false}$ ; *go to* L0

Line 88 becomes:

$\text{cosine} := \text{false}$ ; *go to exit end*;

(iii) To avoid the repeated evaluation of  $F(0)$ ,  $F(1.0)$  the following modification is suggested:

Declare a new variable *term1* of type **real** on line 20.

Replace lines 23 and 24 by:

$\text{term1} := F(1.0) \times \text{cos}(k)$ ;

$\text{sumcos} := (F(0) + \text{term1}) \times 0.5$ ;

$\text{sumsine} := 0$ ;

$\text{term1} := 2 \times (\text{sumcos} - \text{term1})$ ;

Replace lines 44, 45 and 49, 50 by:

$\text{prevint2} := (a \times \text{term1} + b \times \text{sumsine} + g \times \text{oddsine}) \times 0.5$ ;

**begin**  $\text{int2} := h \times (a \times \text{term1} + b \times \text{sumsine} + g \times \text{oddsine})$ ;

Replace lines 76, 77 and 81, 82 by:

$\text{prevint1} := (b \times \text{sumcos} + g \times \text{oddcos}) \times 0.5$ ;

**begin**  $\text{int1} := h \times (b \times \text{sumcos} + g \times \text{oddcos})$ ;

The work described above has been carried out at the National Physical Laboratory.

## CERTIFICATION OF ALGORITHM 296 [E2]

### GENERALIZED LEAST SQUARES FIT BY

### ORTHOGONAL POLYNOMIALS [G. J. Makinson,

*Comm. ACM* 10 (Feb. 1967), 87]

WAYNE T. WATSON (Recd. 11 Feb. 1969 and 21 Mar. 1969)

Service Bureau Corp., Development Laboratory, 111 West St. John Street, San Jose, CA 95113

KEY WORDS AND PHRASES: least squares, curve fitting, orthogonal polynomials, three-term recurrence, polynomial regression, approximation, Forsythe's method

CR CATEGORIES: 5.13, 5.5

LSFITUW was compiled and tested in CALL/360:PL/I. No modifications were made to the algorithm, and the computations were made in long precision (about 15 significant floating point

digits). In addition, *POLYX* [2] was used to transform the results of *LSFITUW* from the interval  $(-2,2)$  to the interval  $(x_1, x_m)$ .

To generally test the algorithm, several small sets of data were used with *LSFITUW* and the results were compared with those obtained from an independently written polynomial curve fitting algorithm which does not use the method of orthogonal polynomials. Only polynomials of degree less than 5 were used to fit the data. Agreement between coefficients and standard errors was good.

As a more comprehensive test of the algorithm, all experiments that could be duplicated from the article by Ascher and Forsythe [1] were performed; a slight modification to *LSFITUW* was required to transform the data to the interval  $(-1,1)$  instead of  $(-2,2)$ . Briefly, the experiments included:

(1) For certain equally spaced data, a comparison of the  $\alpha_i$  and  $\beta_i$  calculated by the program against those values of  $\alpha_i$  and  $\beta_i$  obtained from known formulas ( $\alpha_i=0$  for equally spaced data).

(2) A fit of the function  $f(x) = |x|$  over the interval  $(-1,1)$  for equally spaced data for polynomials of degree as high as 30.

(3) A fit of the function  $f(x) = e^x$  for unequally spaced data inside the interval  $(-1,1)$  for polynomials of degree as high as 32.

The results of experiment (1) showed that *LSFITUW* produced values of  $\beta_i$  differing only in the last significant digit (15) from those calculated by the known formula. The values of  $\alpha_i$  produced were in the range of the floating point round-off error ( $10^{-15}$ ). The results of duplicating experiments (2) and (3) were better than those reported in [1] because of the greater precision used in the calculations (about 10.8 versus about 15 significant floating digits). While conducting the last two experiments, it was noted that for data values of  $x$  symmetric about the origin, the value of  $b$  in the transformation equation  $x = at + b$  may be computed to be a number in the floating point round-off range instead of exactly zero. When fitting polynomials of a sufficiently high degree, this may cause an underflow at line 4 of *POLYX*, the transformation routine. The user may find it desirable to branch on an underflow in *POLYX* and reset  $b$  to zero.

To check the computations of the  $\sigma_k^2$  obtained by the recursive definition of  $\sigma_k^2$  used in the algorithm, the  $\sigma_k^2$  were compared with results computed directly from the equation

$$\sigma_k^2 = \sum_{j=1}^m (f_j - y_k(x_j))^2 / (m - k - 1) \quad (*)$$

where  $y_k$  is the best fitting polynomial of degree  $k$  for the data  $x_j, f_j$ . Experience with the algorithm indicates that a loss of accuracy in computing  $\sigma_k^2$  occurs at smaller values of  $k$  when using the recursive definition than when using (\*). If the values of  $\sigma_k^2$  are of importance to the user, he may find it useful to compute them using (\*) instead.

A comprehensive test of the algorithm's feature which uses the  $\sigma_k^2$  to automatically select the best fitting polynomial was not made, but the feature did work properly for the polynomials used. In connection with this feature, the user should be aware, though, of the possible difficulty mentioned above in computing  $\sigma_k^2$  accurately using the recursive definition. In this case, the user should not expect the algorithm to select the best fitting polynomial. This difficulty was experienced several times while testing the algorithm, but was circumvented by using (\*) to calculate  $\sigma_k^2$ . In order to detect a possible loss in accuracy, the  $\sigma_k^2$  should be examined carefully or compared with those obtained by (\*).

Comprehensive tests were not made using weights; however, no problems were encountered with a moderate usage of this feature.

#### REFERENCES:

1. ASCHER, M., AND FORSYTHE, G. E. SWAC experiments on the use of orthogonal polynomials for data fitting. *J. ACM* 5 (Jan. 1958), 9-21.
2. MACKINNEY, JOHN G. Algorithm 29, Polynomial transformer. *Comm. ACM* 3 (Nov. 1960), 604.

#### 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]

F. K. TOMLIN AND L. B. SMITH (Recd. 17 May 1968, 9 Sept. 1968 and 30 June 1969)

Stanford Research Institute, Menlo Park, CA 94025, and CERN, DD Division, Geneva, Switzerland

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  $\text{maxeval}$ . 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  $\text{maxeval}$  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]

LYLE B. SMITH\* (Recd. 9 Sept. 1968)

Stanford Linear Accelerator Center, Stanford, CA 94305

\* Present address. CERN, Data Handling Division, 1211 Geneva 23, Switzerland

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 <i>f</i>	Final values of the variables		
				X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
For initial values of (0.0, 0.0, 200.0):						
Direct search	66.6667	153	$0.841 \times 10^{-7}$	0.00999995	0.999995	100.000
Modified direct search	.2	112	$0.597 \times 10^{-7}$	0.00999998	0.999990	100.000
For initial values of (0.05, 5.0, 500.0):						
Direct search	168.35	174	$0.934 \times 10^{-7}$	0.0100263	0.998958	99.9999
Modified direct search	.2	75	$0.559 \times 10^{-6}$	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.

#### REMARK ON ALGORITHM 308 [G6]

GENERATION OF PERMUTATIONS IN PSEUDO-LEXICOGRAPHIC ORDER [R. J. Ord-Smith, *Comm. ACM 10* (July 1967), 452]

R. J. ORD-SMITH (Recd. 21 May 1969)

Computing Laboratory, University of Bradford, England

KEY WORDS AND PHRASES: permutations, lexicographic order, lexicographic generation, permutation generation

CR CATEGORIES: 5.39

Following the construction of the very fast lexicographic permutation Algorithm 323 [1] it has become clear that the permutation sequence generated by the Algorithm 308 can be obtained more quickly. In fact, replacement of

```
trstart:m := q[k]; t := x[m]; x[m] := x[k]; x[k] := t;
  q[k] := m + 1; k := k - 1;
```

by

```
trstart: q[k] := q[k] + 1;
```

in Algorithm 323 produces the *ECONOPERM* sequence of Algorithm 308.

The times are as follows on an ICT 1905, in seconds.

	<i>t</i> <sub>1</sub>	<i>t</i> <sub>2</sub>
Algorithm 323	6	47
New <i>ECONOPERM</i>	5.9	45
Old <i>ECONOPERM</i>	6.2	50.6

REFERENCE:

1. ORD-SMITH, R. J. Algorithm 323: Generation of permutations in lexicographic order. *Comm. ACM 11* (Feb. 1968), 117.