

series modification of the classical least squares method is utilized to approximate a solution to the system of nonlinear equations of condition. After every iteration, the statistic E squared is computed as a measure of the goodness of fit. Commencing with the second iteration, the successive values of E squared are differenced, and when the difference in absolute value becomes less than ϵ , the calculations cease. If the number of iterations necessary to achieve this result exceeds l max, a flag is set to a nonzero value and the procedure is terminated. In normal usage, the $jump$ parameter is brought in as a ZERO.

With certain data sets, convergence difficulties will be experienced. In these cases it is sometimes helpful to first utilize the procedure *EXPCRVRT* [Algorithm 275, *Comm. ACM* 9 (Feb. 1966), 85] to obtain initial values for b and c , and then bring the $jump$ parameter in as a ONE in order to bypass the following starting value computations for b and c ;

```

begin
  integer i, l, m;
  real exp factor;
  if jump = 1 then go to entry;
  comment Computation of initial estimates follows;
  b := 2 × ln(abs((y[n] - y[n-1]) × (x[2] - x[1])) /
              ((y[2] - y[1]) × (x[n] - x[n-1]))) /
              (x[n] + x[n-1] - x[2] - x[1]));
  m := (n+1) ÷ 2;
  exp factor := exp(b × (x[m] - x[k]));
  c := (y[m] - z × exp factor) / (1 - exp factor);
  a := (z - c) × exp(-b × x[k]);
  E squared := 0;
  for i := 1 step 1 until n do
    E squared := E squared + (y[i] - c - a × exp(b × x[i])) ↑ 2;
  comment Computation of corrections follows;
entry: for l := 1 step 1 until l max do
  begin
    real sumex1, sumex2, sumqex1, sumqex2, sumqex1lsex2,
          sumq2ex2, sumyi, sumyie1, sumqyie1, zlsc, d11, d12, d22,
          e1, e2, delta, v, w, save;
    sumex1 := sumex2 := sumqex1 := sumqex2 := sumqex1lsex2 :=
      sumq2ex2 := sumyi := sumyie1 := sumqyie1 := 0;
    for i := 1 step 1 until n do
      begin
        real q, ex1, ex2, qex1, qex2, qex1lsex2, q2ex2;
        q := x[i] - x[k];
        ex1 := exp(b × q);
        ex2 := ex1 ↑ 2;
        qex1 := q × ex1;
        qex2 := q × ex2;
        qex1lsex2 := qex1 - qex2;
        q2ex2 := qex2 × q;
        sumex1 := sumex1 + ex1;
        sumex2 := sumex2 + ex2;
        sumqex1 := sumqex1 + qex1;
        sumqex2 := sumqex2 + qex2;
        sumqex1lsex2 := sumqex1lsex2 + qex1lsex2;
        sumq2ex2 := sumq2ex2 + q2ex2;
        sumyi := sumyi + y[i];
        sumyie1 := sumyie1 + ex1 × y[i];
        sumqyie1 := sumqyie1 + qex1 × y[i];
      end
    computation of sum terms in normal equations;
    zlsc := z - c;
    d11 := sumq2ex2 × zlsc ↑ 2;
    d12 := sumqex1lsex2 × zlsc;
    d22 := n - 2 × sumex1 + sumex2;
    e1 := sumqyie1 × zlsc - sumqex2 × zlsc ↑ 2 -
      sumqex1 × zlsc × c;
    e2 := sumyi - sumyie1 + sumex1 × (2 × c - z) +
      sumex2 × zlsc - n × c;
  end
end

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delta := d11 × d22 - d12 ↑ 2;
v := (e1 × d22 - e2 × d12) / delta;
w := (e2 × d11 - e1 × d12) / delta;
b := b + v;
c := c + w;
a := (z - c) × exp(-b × x[k]);
E squared := 0;
for i := 1 step 1 until n do
  E squared := E squared +
    (y[i] - c - a × exp(b × x[i])) ↑ 2;
if l = 1 then go to retry;
if abs(save - E squared) < epsilon
then go to 73
else if l < l max
  then go to retry
  else go to unfurl;
retry: save := E squared;
  end computation of corrected values of a, b, and c;
unfurl: flag := 1;
73: end constrained least squares fit to y = a × exp(b × x) +

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ALGORITHM 277 COMPUTATION OF CHEBYSHEV SERIES COEFFICIENTS [C6]

LYLE B. SMITH (Recd. 15 July 1965, 23 July 1965 and 20
Sept. 1965)

Stanford University, Stanford, California

procedure *CHEBCOEFF* ($F, N, ODD, EVEN, A$);

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  value N;
  Boolean ODD, EVEN;
  integer N;
  real procedure F;
  array A;

```

comment This procedure approximates the first $N+1$ coefficients, a_n , of the infinite Chebyshev series expansion of a function $F(x)$ defined on $[-1, 1]$.

$$F(x) = \sum_{n=0}^{\infty} a_n T_n(x), \quad (1)$$

where \sum' denotes a sum whose first term is halved, and $T_n(x)$ denotes the Chebyshev polynomial of the first kind of degree n , defined by

$$T_n(x) = \cos n\theta, \quad x = \cos \theta \quad (n = 0, 1, 2, \dots).$$

The truncated series $\sum_{n=0}^N a_n T_n(x)$, gives an approximation to $F(x)$ which has maximum error almost as small as that of the "best" polynomial approximation of degree N , see [1]. In this procedure the coefficients, a_n , are closely approximated by $B_{n,N}$, $n = 0(1)N$, which are the coefficients of a "Lagrangian" interpolation polynomial coincident with $F(x)$ at the points x_i , $i = 0(1)N$ where $x_i = \cos(\pi i/N)$, see [2]. The $B_{n,N}$ are given by

$$B_{n,N} = \frac{2}{N} \sum_{i=0}^N{}' F(x_i) T_n(x_i) = \frac{2}{N} \sum_{i=0}^N{}'' F(x_i) T_i(x_n),$$

where \sum'' denotes a sum whose first and last terms are halved. The $B_{n,N}$ are evaluated by a recurrence relation described by Clenshaw in [1] and improved by John Rice [5]. This recurrence relation can also be used to evaluate the truncated series, $\sum_{n=0}^N a_n T_n(x)$, once *CHEBCOEFF* has found values for the coefficients. For even N a relation between $B_{n,N/2}$ and $B_{n,N}$ (pointed out by Clenshaw [3, p. 27]) is used in computing $B_{n,N}$.

For large N , $B_{n,N}$ is very close to a_n . In [2] the relation is given as

$$B_{n,N} = a_n + \sum_{p=1}^{\infty} (a_{2pN-n} + a_{2pN+n}). \quad (2)$$

This shows that $\frac{1}{2}B_{N,N}$ approximates a_N quite well for large N since from (2) we see that

$$\frac{1}{2}B_{N,N} = a_N + a_{3N} + \dots \quad (3)$$

For even N a simple check on the accuracy is available. Since the relation

$$B_{n,N} = B_{n,N/2} - B_{N-n,N}, \quad n = 0(1)N/2-1 \quad (4)$$

is used in the computation, the difference

$$B_{n,N/2} - B_{n,N} = B_{N-n,N}, \quad (5)$$

which measures in some sense the accuracy of the approximation, is available to the user. For instance, in the example below with $N = 8$ the number $A[7]$ is the difference between $A[1]$ for $N = 4$ and $A[1]$ for $N = 8$.

PARAMETER EXPLANATION. If the function F is odd or even then the Boolean parameters *ODD* or *EVEN* should be true respectively in which case every other coefficient in the array A will be zero. The array A will contain the coefficients of the truncated series with $N+1$ terms.

EXAMPLE. For the function $F(x) = e^x$ the following values were computed for $A[n]$ with $N = 4$ and $N = 8$. The computations were done using this procedure written in Extended ALGOL for the Burroughs B5500 computer. Also shown are computed values for the coefficients of the "best" polynomial of degree 8 from [4] (digits differing from the correct result are in italics).

n	$A[n]$ with $N = 4$	$A[n]$ with $N = 8$	"Best" a_n from [4]	Correct a_n from [1]
0	2.53213	<i>21539</i> 2.53213	17555	2.53213 17555
1	1.13032	<i>14175</i> 1.13031	82080	1.13031 82080
2	0.27154	<i>03174</i> 0.27149	53395	0.27149 53395
3	0.04487	<i>97762</i> 0.04433	68498	0.04433 68498
4	0.00547	42404 0.00547	42404	0.00547 42404
5		0.00054	29263	0.00054 29263
6		0.00004	49779	0.00004 49773
7		0.00000	<i>32095</i> 0.00000	31984 0.00000 31984
8		0.00000	01992	0.00000 01998

begin

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integer i, m, N2, S1, S2, T1;
real b0, b1, b2, pi, TWOX, FXN2;
array FX, X[0:N];
Boolean TEST;
pi := 3.14159265359;
N2 := N ÷ 2;
comment If N is even TEST is set to true;
if 2 × N2 = N then TEST := true
else TEST := false;
comment Compute the necessary function values;
for i := 0 step 1 until N do
begin
  X[i] := cos(pi × i/N);
  FX[i] := F(X[i]);
end;
S2 := 1; S1 := 0;
comment If F(x) is odd or even initialize accordingly;
if ODD then
begin
  for m := 0 step 2 until N do
    A[m] := 0;
  S2 := 2; S1 := 1;
end else

```

if EVEN then

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begin
  for m := 1 step 2 until N do
    A[m] := 0;
  S2 := 2; S1 := 0;
end;
comment If TEST is true the coefficients are computed in
two steps;
FXN2 := FX[N]/2.0;
if TEST then
begin
  for m := S1 step S2 until N2 do
  begin
    b1 := 0;
    b0 := FXN2;
    TWOX := 2.0 × X[2 × m];
    for i := N-2 step -2 until 2 do
    begin
      b2 := b1; b1 := b0;
      b0 := TWOX × b1 - b2 + FX[i];
    end;
    A[m] := 2.0 × (X[2×m]×b0 - b1 + FX[0]/2.0)/N2;
  end;
  A[N2] := A[N2]/2.0;
  T1 := S1;
  if ODD ∨ EVEN then
  begin
    if 2 × (N2 ÷ 2) = N2
    then S1 := N2 + 2 - S1
    else S1 := N2 + 1 + S1;
  end
  else S1 := N2 + 1;
end;
comment Compute the desired coefficients;
for m := S1 step S2 until N do
begin
  b1 := 0;
  b0 := FXN2;
  TWOX := 2.0 × X[m];
  for i := N-1 step -1 until 1 do
  begin
    b2 := b1; b1 := b0;
    b0 := TWOX × b1 - b2 + FX[i];
  end;
  A[m] := 2.0 × (X[m]×b0 - b1 + FX[0]/2.0)/N;
end;
if TEST then
begin
  for i := T1 step S2 until N2-1 do
    A[i] := A[i] - A[N-i];
end;
A[N] := A[N]/2.0;
end CHEBCOEFF

```

REFERENCES:

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2. ELLIOTT, D. Truncation errors in two Chebyshev series approximations. *Math. Comp.* 19 (1965), 234-248.
3. CLENSHAW, C. W. A comparison of "best" polynomial approximations with truncated Chebyshev series expansions. *J. SIAM* {B}, 1 (1964), 26-37.
4. Computed values by Dr. C. L. Lawson. (private communication)
5. RICE, JOHN. On the conditioning of polynomials and rational forms. (submitted for publication).

ALGORITHM 278

GRAPH PLOTTER [J6]

P. LLOYD (Recd. 4 June 1965)

Queen Mary College, London, England

```

procedure graphplotter (N, x, y, m, n, xerror, yerror, g, L, S, EM,
    C0, C1, C2, C3, C4, label);
    value N, m, n, xerror, yerror, g, L, S;
    array x, y;
    integer N, g, m, n, L, S;
    real xerror, yerror;
    string EM, C0, C1, C2, C3, C4;
    label label;

```

comment This procedure is intended to be used to give an approximate graphical display of a multivalued function, $y[i, j]$ of $x[i]$, on a line printer. Output channel N is selected for all output from *graphplotter*. The display is confined to points for which $1 \leq i \leq m$ and $1 \leq j \leq n$ where $2 \leq n \leq 4$. If $n = 1$, then y is considered to be a one-dimensional array $y[i]$ and the display is again given for $1 \leq i \leq m$. The format of the print out is arranged so that a margin of g spaces separates the display from the left-hand side of the page. L and S denote the number of lines down the page and the number of spaces across the page which the display will occupy. The graph is plotted so that lines 1 and L correspond to the minimum and maximum values of x , and the spaces 1 and S correspond to the minimum and maximum values of y , that is, y is plotted across the page and x down the page. After the graph has been plotted, the ranges of x and y for which the display is given are printed out in the order as above, separated from the display by a blank line. The strings *EM* ... *C4* must be such that they occupy only one character position when printed out. The characters of *C1 C2 C3 C4* represent $y[i,1]$ $y[i,2]$ $y[i,3]$ $y[i,4]$. *EM* is the character printed out round the perimeter of the display. *C0* is printed at empty positions. At coincident points the order of precedence of the characters is *C1 C2 C3 C4 EM C0*. For the special case $n=1$ the character *C1* represents $y[i]$. Control is passed from the procedure to the point labeled *label* if the interval between the maximum value and minimum values of $x[i]$ is less than *xerror*, or if the range of y is less than *yerror*. If the values of $x[i]$ occur at equal intervals, choosing $L=m$ will make one line equivalent to one interval of x ;

```

begin
    real p, q, xmax, xmin, ymax, ymin;
    integer i, j;
    integer array plot[1:L,1:S];
    xmax := xmin := x[1];
    for i := 2 step 1 until m do
        begin
            if x[i] > xmax then xmax := x[i];
            if x[i] < xmin then xmin := x[i];
        end of hunt for maximum and minimum values of x;
        if n=1 then go to N1A;
        ymax := ymin := y[1,1];
        for i := 1 step 1 until m do
            for j := 1 step 1 until n do
                begin
                    if y[i,j] > ymax then ymax := y[i,j];
                    if y[i,j] < ymin then ymin := y[i,j];
                end of hunt for maximum and minimum values of y;
            escape: if  $\text{abs}(x_{\text{max}} - x_{\text{min}}) < x_{\text{error}} \vee \text{abs}(y_{\text{max}} - y_{\text{min}}) < y_{\text{error}}$  then go to label;
            p := (L-1)/(xmax-xmin); q := (S-1)/(ymax-ymin);
            for i := 1 step 1 until L do
                for j := 1 step 1 until S do plot[i,j] := 2;
            for i := 1, L do

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        for j := 1 step 1 until S do plot[i,j] := 1;
        for i := 2 step 1 until L-1 do
            for j := 1, S do plot[i,j] := 1;
        if n = 1 then go to N1B;
        for i := 1 step 1 until m do
            for j := n step -1 until 1 do
                plot[1+entier(0.5+p×(x[i]-xmin)),
                    1+entier(0.5+q×(y[i,j]-ymin))] := j+2;
        plotter:
        for i := 1 step 1 until L do
            begin
                NEWLINE(N,1); SPACE(N,g);
                comment NEWLINE and SPACE must be declared globally to graphplotter, NEWLINE(N,p) outputs p carriage returns and p line feeds on channel N, SPACE(N,p) outputs p blank character positions on channel N;
                for j := 1 step 1 until S do
                    begin
                        switch SW := SW1, SW2, SW3, SW4, SW5, SW6;
                        go to SW[plot[i,j]];
                    SW1: outstring(N,EM); go to fin;
                    SW2: outstring(N,C0); go to fin;
                    SW3: outstring(N,C1); go to fin;
                    SW4: outstring(N,C2); go to fin;
                    SW5: outstring(N,C3); go to fin;
                    SW6: outstring(N,C4);
                fin:
                    end
            end of display output;
            NEWLINE(N,2); SPACE(N,g); outreal(N,xmin);
            outreal(N,xmax);
            outreal(N,ymin); outreal(N,ymax);
            go to end;
        N1A:
            ymax := ymin := y[1];
            for i := 2 step 1 until m do
                begin
                    if y[i] > ymax then ymax := y[i];
                    if y[i] < ymin then ymin := y[i];
                end of hunt for maximum and minimum values of y when
                n = 1;
                go to escape;
        N1B:
            for i := 1 step 1 until m do
                plot[1+entier(0.5+p×(x[i]-xmin)),
                    1+entier(0.5+q×(y[i]-ymin))] := 3;
                go to plotter;
            end:
        end of graphplotter

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1966 CONFERENCE DATES

ACM SYMSAM	March 29-31	WASHINGTON
SPRING JCC	April 26-28	BOSTON
ACM 66	August 30-Sept. 1	LOS ANGELES
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