

NAG Fortran Library Routine Document

E02AFF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details.

1 Purpose

E02AFF computes the coefficients of a polynomial, in its Chebyshev-series form, which interpolates (passes exactly through) data at a special set of points. Least-squares polynomial approximations can also be obtained.

2 Specification

```
SUBROUTINE E02AFF(NPLUS1, F, A, IFAIL)
INTEGER          NPLUS1, IFAIL
real           F(NPLUS1), A(NPLUS1)
```

3 Description

This routine computes the coefficients a_j , for $j = 1, 2, \dots, n + 1$, in the Chebyshev-series

$$\frac{1}{2}a_1T_0(\bar{x}) + a_2T_1(\bar{x}) + a_3T_2(\bar{x}) + \dots + a_{n+1}T_n(\bar{x}),$$

which interpolates the data f_r at the points

$$\bar{x}_r = \cos((r - 1)\pi/n), \quad r = 1, 2, \dots, n + 1.$$

Here $T_j(\bar{x})$ denotes the Chebyshev polynomial of the first kind of degree j with argument \bar{x} . The use of these points minimizes the risk of unwanted fluctuations in the polynomial and is recommended when the data abscissae can be chosen by the user, e.g., when the data is given as a graph. For further advantages of this choice of points, see Clenshaw (1962).

In terms of the user's original variables, x say, the values of x at which the data f_r are to be provided are

$$x_r = \frac{1}{2}(x_{\max} - x_{\min}) \cos(\pi(r - 1)/n) + \frac{1}{2}(x_{\max} + x_{\min}), \quad r = 1, 2, \dots, n + 1$$

where x_{\max} and x_{\min} are respectively the upper and lower ends of the range of x over which the user wishes to interpolate.

Truncation of the resulting series after the term involving a_{i+1} , say, yields a least-squares approximation to the data. This approximation, $p(\bar{x})$, say, is the polynomial of degree i which minimizes

$$\frac{1}{2}\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2 + \dots + \epsilon_n^2 + \frac{1}{2}\epsilon_{n+1}^2,$$

where the residual $\epsilon_r = p(\bar{x}_r) - f_r$, for $r = 1, 2, \dots, n + 1$.

The method employed is based on the application of the three-term recurrence relation due to Clenshaw (1955) for the evaluation of the defining expression for the Chebyshev coefficients (see, for example, Clenshaw (1962)). The modifications to this recurrence relation suggested by Reinsch and Gentleman (see Gentleman (1969)) are used to give greater numerical stability.

For further details of the algorithm and its use see Cox (1974) and Cox and Hayes (1973).

Subsequent evaluation of the computed polynomial, perhaps truncated after an appropriate number of terms, should be carried out using E02AEF.

4 References

Clenshaw C W (1955) A note on the summation of Chebyshev-series *Math. Tables Aids Comput.* **9** 118–120

Clenshaw C W (1962) Mathematical tables *Chebyshev-series for Mathematical Functions* HMSO

Cox M G (1974) A data-fitting package for the non-specialist user *Software for Numerical Mathematics* (ed D J Evans) Academic Press

Cox M G and Hayes J G (1973) Curve fitting: a guide and suite of algorithms for the non-specialist user *NPL Report NAC26* National Physical Laboratory

Gentleman W M (1969) An error analysis of Goertzel's (Watt's) method for computing Fourier coefficients *Comput. J.* **12** 160–165

5 Parameters

1: NPLUS1 – INTEGER *Input*

On entry: the number $n + 1$ of data points (one greater than the degree n of the interpolating polynomial).

Constraint: $NPLUS1 \geq 2$.

2: F(NPLUS1) – *real* array *Input*

On entry: for $r = 1, 2, \dots, n + 1$, $F(r)$ must contain f_r the value of the dependent variable (ordinate) corresponding to the value

$$\bar{x}_r = \cos(\pi(r - 1)/n)$$

of the independent variable (abscissa) \bar{x} , or equivalently to the value

$$x(r) = \frac{1}{2}(x_{\max} - x_{\min}) \cos(\pi(r - 1)/n) + \frac{1}{2}(x_{\max} + x_{\min})$$

of the user's original variable x . Here x_{\max} and x_{\min} are respectively the upper and lower ends of the range over which the user wishes to interpolate.

3: A(NPLUS1) – *real* array *Output*

On exit: $A(j)$ is the coefficient a_j in the interpolating polynomial, for $j = 1, 2, \dots, n + 1$.

4: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: $IFAIL = 0$ unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry $IFAIL = 0$ or -1 , explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, $NPLUS1 < 2$.

7 Accuracy

The rounding errors committed are such that the computed coefficients are exact for a slightly perturbed set of ordinates $f_r + \delta f_r$. The ratio of the sum of the absolute values of the δf_r to the sum of the absolute values of the f_r is less than a small multiple of $(n + 1)\epsilon$, where ϵ is the *machine precision*.

8 Further Comments

The time taken by the routine is approximately proportional to $(n + 1)^2 + 30$.

For choice of degree when using the routine for least-squares approximation, see Section 3.2 of the E02 Chapter Introduction.

9 Example

Determine the Chebyshev coefficients of the polynomial which interpolates the data \bar{x}_r, f_r , for $r = 1, 2, \dots, 11$, where $\bar{x}_r = \cos(\pi \times (r - 1)/10)$ and $f_r = e^{\bar{x}_r}$. Evaluate, for comparison with the values of f_r , the resulting Chebyshev series at \bar{x}_r , for $r = 1, 2, \dots, 11$.

The example program supplied is written in a general form that will enable polynomial interpolations of arbitrary data at the cosine points $\cos(\pi \times (r - 1)/n)$, for $r = 1, 2, \dots, n + 1$ to be obtained for any n ($= \text{NPLUS1} - 1$). Note that E02AEF is used to evaluate the interpolating polynomial. The program is self-starting in that any number of data sets can be supplied.

9.1 Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      E02AFF Example Program Text
*      Mark 14 Revised.  NAG Copyright 1989.
*      .. Parameters ..
INTEGER          NMAX, NP1MAX
PARAMETER        (NMAX=199, NP1MAX=NMAX+1)
INTEGER          NIN, NOUT
PARAMETER        (NIN=5, NOUT=6)
*      .. Local Scalars ..
real           FIT, PI, PIBY2N
INTEGER          I, IFAIL, J, N, R
*      .. Local Arrays ..
real           AN(NP1MAX), F(NP1MAX), XCAP(NP1MAX)
*      .. External Functions ..
real           X01AAF
EXTERNAL         X01AAF
*      .. External Subroutines ..
EXTERNAL         E02AEF, E02AFF
*      .. Intrinsic Functions ..
INTRINSIC       real, SIN
*      .. Executable Statements ..
WRITE (NOUT,*) 'E02AFF Example Program Results'
*      Skip heading in data file
READ (NIN,*)
PI = X01AAF(PI)
20 READ (NIN,*,END=80) N
IF (N.GT.0 .AND. N.LE.NMAX) THEN
  PIBY2N = 0.5e0*PI/real(N)
  READ (NIN,*) (F(R),R=1,N+1)
  DO 40 R = 1, N + 1
    I = R - 1
*
*      The following method of evaluating XCAP = cos(PI*I/N)
*      ensures that the computed value has a small relative error
*      and, moreover, is bounded in modulus by unity for all
*      I = 0, 1, ..., N. (It is assumed that the sine routine
*      produces a result with a small relative error for values
```

```

*           of the argument between  $-\pi/4$  and  $\pi/4$ ).
*
      IF (4*I.LE.N) THEN
        XCAP(I+1) = 1.0e0 - 2.0e0*SIN(PIBY2N*I)**2
      ELSE IF (4*I.GT.3*N) THEN
        XCAP(I+1) = 2.0e0*SIN(PIBY2N*(N-I))**2 - 1.0e0
      ELSE
        XCAP(I+1) = SIN(PIBY2N*(N-2*I))
      END IF
40    CONTINUE
      IFAIL = 0
*
      CALL E02AFF(N+1,F,AN,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) '           Chebyshev'
      WRITE (NOUT,*) ' J   coefficient A(J)'
      WRITE (NOUT,99998) (J,AN(J),J=1,N+1)
      WRITE (NOUT,*)
      WRITE (NOUT,*) ' R   Abscissa   Ordinate   Fit'
      DO 60 R = 1, N + 1
        IFAIL = 0
*
        CALL E02AEF(N+1,AN,XCAP(R),FIT,IFAIL)
*
        WRITE (NOUT,99999) R, XCAP(R), F(R), FIT
60    CONTINUE
      GO TO 20
      END IF
80    STOP
*
99999 FORMAT (1X,I3,3F11.4)
99998 FORMAT (1X,I3,F14.7)
      END

```

9.2 Program Data

E02AFF Example Program Data

```

10
2.7182
2.5884
2.2456
1.7999
1.3620
1.0000
0.7341
0.5555
0.4452
0.3863
0.3678

```

9.3 Program Results

E02AFF Example Program Results

```

           Chebyshev
J   coefficient A(J)
1   2.5320000
2   1.1303095
3   0.2714893
4   0.0443462
5   0.0055004
6   0.0005400
7   0.0000307
8   -0.0000006
9   -0.0000004
10  0.0000049
11  -0.0000200

R   Abscissa   Ordinate   Fit

```

1	1.0000	2.7182	2.7182
2	0.9511	2.5884	2.5884
3	0.8090	2.2456	2.2456
4	0.5878	1.7999	1.7999
5	0.3090	1.3620	1.3620
6	0.0000	1.0000	1.0000
7	-0.3090	0.7341	0.7341
8	-0.5878	0.5555	0.5555
9	-0.8090	0.4452	0.4452
10	-0.9511	0.3863	0.3863
11	-1.0000	0.3678	0.3678
