NAG Fortran Library Routine Document

F03ABF

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

F03ABF calculates the determinant of a real symmetric positive-definite matrix using a Cholesky factorization.

2   Specification

```
SUBROUTINE F03ABF(A, IA, N, DET, WKSPCE, IFAIL)
INTEGER          IA, N, IFAIL
real             A(IA,*), DET, WKSPCE(*)
```

3   Description

The determinant of A is calculated using the Cholesky factorization $A = LL^T$, where L is lower triangular. The determinant of A is the product of the squares of the diagonal elements of L.

4   References

Wilkinson J H and Reinsch C (1971) *Handbook for Automatic Computation II, Linear Algebra* Springer-Verlag

5   Parameters

1:    A(IA,*) – **real** array   *Input/Output*

    Note: the second dimension of the array A must be at least $\max(1, N)$.

    On entry: the upper triangle of the n by n positive-definite symmetric matrix A. The elements of the array below the diagonal need not be set.

    On exit: the sub-diagonal elements of the lower triangular matrix L. The upper triangle of A is unchanged.

2:    IA – INTEGER   *Input*

    On entry: the first dimension of the array A as declared in the (sub)program from which F03ABF is called.

    Constraint: $\text{IA} \geq \max(1, N)$.

3:    N – INTEGER   *Input*

    On entry: n, the order of the matrix A.

    Constraint: $N \geq 0$.

4:    DET – **real**   *Output*

    On exit: the determinant of A.

5:    WKSPCE(*) – **real** array   *Workspace*

    Note: the dimension of the array WKSPCE must be at least $\max(1, N)$.

6:     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

The matrix A is not positive-definite, possibly due to rounding errors. The factorization could not be completed. DET is set to 0.0.

IFAIL = 2

Overflow. The value of the determinant is too large to be held in the computer.

IFAIL = 3

Underflow. The value of the determinant is too small to be held in the computer.

IFAIL = 4

On entry, N < 0,
or   IA < max(1, N).

7   Accuracy

The accuracy of the determinant depends on the conditioning of the original matrix. For a detailed error analysis see page 25 of Wilkinson and Reinsch (1971).

8   Further Comments

The time taken by the routine is approximately proportional to n^3.

9   Example

To calculate the determinant of the real symmetric positive-definite matrix

$$\begin{pmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{pmatrix}.$$

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.

```
*      F03ABF Example Program Text
*      Mark 15 Revised.  NAG Copyright 1991.
*      .. Parameters ..
       INTEGER          NMAX, IA
       PARAMETER        (NMAX=8,IA=NMAX)
       INTEGER          NIN, NOUT
       PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
       real             DETERM
       INTEGER          I, IFAIL, J, N
*      .. Local Arrays ..
       real             A(IA,NMAX), WKSPCE(NMAX)
*      .. External Subroutines ..
       EXTERNAL         F03ABF
*      .. Executable Statements ..
       WRITE (NOUT,*) 'F03ABF Example Program Results'
*      Skip heading in data file
       READ (NIN,*)
       READ (NIN,*) N
       WRITE (NOUT,*)
       IF (N.GE.0 .AND. N.LE.NMAX) THEN
          READ (NIN,*) ((A(I,J),J=1,N),I=1,N)
          IFAIL = 0
*
          CALL F03ABF(A,IA,N,DETERM,WKSPCE,IFAIL)
*
          WRITE (NOUT,99998) 'Value of determinant = ', DETERM
       ELSE
          WRITE (NOUT,99999) 'N is out of range: N = ', N
       END IF
       STOP
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,A,F9.4)
       END
```

9.2 Program Data

```
F03ABF Example Program Data
  4
    5    7    6    5
    7   10    8    7
    6    8   10    9
    5    7    9   10
```

9.3 Program Results

```
 F03ABF Example Program Results

 Value of determinant =    1.0000
```