

## F03ABF – NAG Fortran Library Routine Document

**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

- [1] 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:*  $IA \geq \max(1,N)$ .
- 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. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

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

**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 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 Wilkinson and Reinsch [1] page 25.

**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

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