NAG Fortran Library Routine Document

F01ABF

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

F01ABF calculates the accurate inverse of a real symmetric positive-definite matrix, using a Cholesky factorization and iterative refinement.

2 Specification

```
SUBROUTINE F01ABF(A, IA, N, B, IB, Z, IFAIL)
INTEGER           IA, N, IB, IFAIL
real              A(IA,N), B(IB,N), Z(N)
```

3 Description

To compute the inverse X of a real symmetric positive-definite matrix A, this routine first computes a Cholesky factorization of A as $A = LL^T$, where L is lower triangular. An approximation to X is found by computing L^{-1} and then the product $(L^{-1})^T L^{-1}$. The residual matrix $R = I - AX$ is calculated using ***additional precision***, and a correction D to X is found by solving $LL^T D = R$. X is replaced by $X + D$, and this iterative refinement of the inverse is repeated until full machine accuracy has been obtained.

4 References

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

5 Parameters

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

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 lower triangle of the inverse matrix X is stored in the elements of the array below the diagonal, in rows 2 to $n+1$; x_{ij} is stored in A$(i+1, j)$ for $i \geq j$. The upper triangle of the original matrix is unchanged.

2: IA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01ABF is called.

Constraint: IA $\geq$ N + 1.

3: N – INTEGER *Input*

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

Constraint: N ≥ 1.

4: B(IB,N) – ***real*** array *Output*

On exit: the lower triangle of the inverse matrix X, with x_{ij} stored in B(i, j), for $i \geq j$.

5: IB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F01ABF is called.

Constraint: IB $\geq$ N.

6: Z(N) – ***real*** array *Workspace*

7: 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.

IFAIL $= 2$

The refinement process fails to converge, i.e., the matrix A is ill-conditioned.

7 Accuracy

The computed inverse should be correct to full machine accuracy. For a detailed error analysis see page 40 of Wilkinson and Reinsch (1971).

8 Further Comments

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

9 Example

To find the inverse of the 4 by 4 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.

```
*     F01ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX, IA, IB
      PARAMETER        (NMAX=8,IA=NMAX+1,IB=NMAX)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, N
*     .. Local Arrays ..
      real             A(IA,NMAX), B(IB,NMAX), Z(NMAX)
*     .. External Subroutines ..
      EXTERNAL         F01ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F01ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      WRITE (NOUT,*)
      IF (N.GT.0 .AND. N.LE.NMAX) THEN
         READ (NIN,*) ((A(I,J),J=1,N),I=1,N)
         IFAIL = 1
*
         CALL F01ABF(A,IA,N,B,IB,Z,IFAIL)
*
         IF (IFAIL.NE.0) THEN
            WRITE (NOUT,99999) 'Error in F01ABF. IFAIL =', IFAIL
         ELSE
            WRITE (NOUT,*) 'Lower triangle of inverse'
            DO 20 I = 1, N
               WRITE (NOUT,99998) (B(I,J),J=1,I)
   20       CONTINUE
         END IF
      ELSE
         WRITE (NOUT,99999) 'N is out of range: N = ', N
      END IF
      STOP
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,8F9.4)
      END
```

9.2 Program Data

```
F01ABF Example Program Data
  4
   5.   7.   6.   5.
   7.  10.   8.   7.
   6.   8.  10.   9.
   5.   7.   9.  10.
```

9.3 Program Results

```
 F01ABF Example Program Results

 Lower triangle of inverse
   68.0000
  -41.0000  25.0000
  -17.0000  10.0000   5.0000
   10.0000  -6.0000  -3.0000   2.0000
```