NAG Fortran Library Routine Document

F01ADF

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

F01ADF calculates the approximate inverse of a real symmetric positive-definite matrix, using a Cholesky factorization.

2 Specification

```
SUBROUTINE F01ADF (N, A, IA, IFAIL)
INTEGER            N, IA, IFAIL
double precision   A(IA,*)
```

3 Description

To compute the inverse X of a real symmetric positive-definite matrix A, F01ADF first computes a Cholesky factorization of A as $A = LL^{\mathrm{T}}$, where L is lower triangular. It then computes L^{-1} and finally forms X as the product $L^{-\mathrm{T}}L^{-1}$.

4 References

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

5 Parameters

1: N – INTEGER *Input*

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

Constraint: $\mathrm{N} \geq 0$.

2: A(IA,$*$) – ***double precision*** array *Input/Output*

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

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 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 $\mathrm{A}(i+1,j)$ for $i \geq j$. The upper triangle of the original matrix is unchanged.

3: IA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01ADF is called.

Constraint: $\mathrm{IA} \geq \mathrm{N} + 1$.

4: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you 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, if you are 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 $= 2$

On entry, N < 0,
or IA $<$ N $+ 1$.

7 Accuracy

The accuracy of the computed inverse depends on the conditioning of the original matrix. For a detailed error analysis see page 39 of Wilkinson and Reinsch (1971).

8 Further Comments

The time taken by F01ADF is approximately proportional to n^3. F01ADF calls routines F07FDF (DPOTRF) and F07FJF (DPOTRI) from LAPACK.

9 Example

This example finds 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

```
*     F01ADF Example Program Text
*     Mark 15 Revised. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NMAX, IA
      PARAMETER        (NMAX=8,IA=NMAX+1)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, N
*     .. Local Arrays ..
      DOUBLE PRECISION A(IA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         F01ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F01ADF 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 F01ADF(N,A,IA,IFAIL)
*
         WRITE (NOUT,*) 'Lower triangle of inverse'
         DO 20 I = 1, N
            WRITE (NOUT,99998) (A(I+1,J),J=1,I)
   20    CONTINUE
      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

```
F01ADF Example Program Data
  4
   5.   7.   6.   5.
   7.  10.   8.   7.
   6.   8.  10.   9.
   5.   7.   9.  10.
```

9.3 Program Results

```
 F01ADF 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
```