

NAG 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, LDA, IFAIL)
INTEGER          N, LDA, IFAIL
double precision A(LDA,*)
```

3 Description

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

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: $N \geq 0$.
- 2: A(LDA,*) – **double precision** 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 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.
- 3: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F01ADF is called.
Constraint: $LDA \geq N + 1$.
- 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 Section 3.3 in the Essential Introduction 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 LDA $< N + 1$.

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, LDA
      PARAMETER        (NMAX=8,LDA=NMAX+1)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      INTEGER          I, IFAIL, J, N
*      .. Local Arrays ..
      DOUBLE PRECISION A(LDA,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 = 1
*
        CALL F01ADF(N,A,LDA,IFAIL)
*
        IF (IFAIL.EQ.0) THEN
          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,99997) IFAIL
          END IF
        ELSE
          WRITE (NOUT,99999) 'N is out of range: N = ', N
        END IF
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,8F9.4)
99997 FORMAT (1X,/1X,' ** F01ADF returned with IFAIL = ',I5)
      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

```
