F01ADF - 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

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

2 Specification

SUBROUTINE FO1ADF(N, A, IA, IFAIL)
INTEGER N, IA, IFAIL

real A(IA,*)

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. It then computes L^{-1} and finally forms X as the product $(L^{-1})^T L^{-1}$.

4 References

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

5 Parameters

1: N — INTEGER

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

Constraint: $N \geq 0$.

2: 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 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: IA — INTEGER Input

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

Constraint: IA \geq N + 1.

4: 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).

[NP3390/19/pdf] F01ADF.1

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.

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 Wilkinson and Reinsch [1] page 39.

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.

```
FO1ADF Example Program Text
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.. 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 ..
real
                 A(IA, NMAX)
.. External Subroutines ..
EXTERNAL
                 F01ADF
.. Executable Statements ...
WRITE (NOUT,*) 'FO1ADF Example Program Results'
Skip heading in data file
READ (NIN,*)
READ (NIN,*) N
WRITE (NOUT,*)
IF (N.GE.O .AND. N.LE.NMAX) THEN
```

F01ADF.2 [NP3390/19/pdf]

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

FO1ADF 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
```

[NP3390/19/pdf] F01ADF.3 (last)