NAG Fortran Library Routine Document

F01BUF

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

F01BUF performs a $ULDL^TU^T$ decomposition of a real symmetric positive-definite band matrix.

2 Specification

```
SUBROUTINE F01BUF(N, M1, K, A, IA, W, IFAIL)
INTEGER            N, M1, K, IA, IFAIL
real               A(IA,N), W(M1)
```

3 Description

The symmetric positive-definite matrix A, of order n and bandwidth $2m+1$, is divided into the leading principal sub-matrix of order k and its complement, where $m \leq k \leq n$. A UDU^T decomposition of the latter and an LDL^T decomposition of the former are obtained by means of a sequence of elementary transformations, where U is unit upper triangular, L is unit lower triangular and D is diagonal. Thus if $k = n$, an LDL^T decomposition of A is obtained.

This routine is specifically designed to precede F01BVF for the transformation of the symmetric-definite eigenproblem $Ax = \lambda Bx$ by the method of Crawford where A and B are of band form. In this context, k is chosen to be close to $n/2$ and the decomposition is applied to the matrix B.

4 References

Wilkinson J H (1965) *The Algebraic Eigenvalue Problem* Oxford University Press, Oxford

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.

2: M1 – INTEGER *Input*

On entry: $m+1$, where m is the number of non-zero super-diagonals in A. Normally M1 $\ll$ N.

3: K – INTEGER *Input*

On entry: k, the change-over point in the decomposition.

Constraint: M $-$ 1 $\leq$ K $\leq$ N.

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

On entry: the upper triangle of the n by n symmetric band matrix A, with the diagonal of the matrix stored in the $(m+1)$th row of the array, and the m super-diagonals within the band stored in the first m rows of the array. Each column of the matrix is stored in the corresponding column of the array. For example, if $n = 6$ and $m = 2$, the storage scheme is

$$\begin{array}{cccccc} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \end{array}$$

Elements in the top left corner of the array are not used. The following code assigns the matrix elements within the band to the correct elements of the array:

```
  DO 20 J = 1, N
     DO 10 I = MAX(1,J-M1+1), J
        A(I-J+M1,J) = matrix (I,J)
10   CONTINUE
20 CONTINUE
```

On exit: A is overwritten by the corresponding elements of L, D and U.

5: IA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01BUF is called.

Constraint: IA $\geq$ M1.

6: W(M1) – ***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 $= 1$

On entry, K $<$ M or K $>$ N.

IFAIL $= 2$

The matrix A is not positive-definite, perhaps as a result of rounding errors, giving an element of D which is zero or negative. IFAIL=3 when the failure occurs in the leading principal sub-matrix of order K and IFAIL $= 2$ when it occurs in the complement.

7 Accuracy

The Cholesky decomposition of a positive-definite matrix is known for its remarkable numerical stability (see Wilkinson (1965)). The computed U, L and D satisfy the relation $ULDL^TU^T = A + E$ where the 2-norms of A and E are related by $\|E\| \leq c(m+1)^2\epsilon\|A\|$ where c is a constant of order unity and ϵ is the ***machine precision***. In practice, the error is usually appreciably smaller than this.

8 Further Comments

The time taken by the routine is approximately proportional to $nm^2 + 3nm$.

This routine is specifically designed for use as the first stage in the solution of the generalized symmetric eigenproblem $Ax = \lambda Bx$ by Crawford's method which preserves band form in the transformation to a similar standard problem. In this context, for maximum efficiency, k should be chosen as the multiple of m nearest to $n/2$.

The matrix U is such that $U^{-1}AU^{-T}$ is diagonal in its last $n-k$ rows and columns, L is such that $L^{-1}U^{-1}AU^{-T}L^{-T} = D$ and D is diagonal. To find U, L and D where $A = ULDL^TU^T$ requires $nm(m+3)/2 - m(m+1)(m+2)/3$ multiplications and divisions which, is independent of k.

9 Example

To find a $ULDL^TU^T$ decomposition of the real symmetric positive-definite matrix

$$\begin{pmatrix} 3 & -9 & 6 & & & & \\ -9 & 31 & -2 & -4 & & & \\ 6 & -2 & 123 & -66 & 15 & & \\ & -4 & -66 & 145 & -24 & 4 & \\ & & 15 & -24 & 61 & -74 & -18 \\ & & & 4 & -74 & 98 & 24 \\ & & & & -18 & 24 & 6 \end{pmatrix}.$$

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.

```
*     F01BUF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX, M1MAX, IA
      PARAMETER        (NMAX=20,M1MAX=8,IA=M1MAX)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, K, M, M1, N
*     .. Local Arrays ..
      real             A(IA,NMAX), W(M1MAX)
*     .. External Subroutines ..
      EXTERNAL         F01BUF
*     .. Intrinsic Functions ..
      INTRINSIC        MAX
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F01BUF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, M1
      IF (N.GT.0 .AND. N.LE.NMAX .AND. M1.GT.0 .AND. M1.LE.M1MAX) THEN
         READ (NIN,*) ((A(J,I),J=MAX(1,M1+1-I),M1),I=1,N)
         M = M1 - 1
         K = ((N+M)/(2*M))*M
         IFAIL = 0
*
         CALL F01BUF(N,M1,K,A,IA,W,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Computed upper triangular matrix'
         WRITE (NOUT,*)
         DO 20 I = 1, N
            WRITE (NOUT,99999) (A(J,I),J=MAX(1,M1+1-I),M1)
   20    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,8F9.4)
      END
```

9.2 Program Data

```
F01BUF Example Program Data
  7  3
     3
    -9    31
     6    -2   123
    -4   -66   145
    15   -24    61
     4   -74    98
   -18    24     6
```

9.3 Program Results

```
 F01BUF Example Program Results

 Computed upper triangular matrix

    3.0000
   -3.0000   4.0000
    2.0000   4.0000   2.0000
   -1.0000   5.0000   3.0000
    3.0000  -4.0000   5.0000
    2.0000  -1.0000   2.0000
   -3.0000   4.0000   6.0000
```