NAG Library Routine Document

F07HAF (DPBSV)

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

F07HAF (DPBSV) computes the solution to a real system of linear equations

$$AX = B,$$

where A is an n by n symmetric positive definite band matrix of bandwidth $(2k_d + 1)$ and X and B are n by r matrices.

2 Specification

```
SUBROUTINE F07HAF (UPLO, N, KD, NRHS, AB, LDAB, B, LDB, INFO)

INTEGER              N, KD, NRHS, LDAB, LDB, INFO
REAL (KIND=nag_wp)   AB(LDAB,*), B(LDB,*)
CHARACTER(1)         UPLO
```

The routine may be called by its LAPACK name ***dpbsv***.

3 Description

F07HAF (DPBSV) uses the Cholesky decomposition to factor A as $A = U^{\mathrm{T}}U$ if UPLO = 'U' or $A = LL^{\mathrm{T}}$ if UPLO = 'L', where U is an upper triangular band matrix, and L is a lower triangular band matrix, with the same number of superdiagonals or subdiagonals as A. The factored form of A is then used to solve the system of equations $AX = B$.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia http://www.netlib.org/lapack/lug

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: UPLO – CHARACTER(1) *Input*

On entry: if UPLO = 'U', the upper triangle of A is stored.

If UPLO = 'L', the lower triangle of A is stored.

Constraint: UPLO = 'U' or 'L'.

2: N – INTEGER *Input*

On entry: n, the number of linear equations, i.e., the order of the matrix A.

Constraint: N ≥ 0.

3: KD – INTEGER *Input*

On entry: k_d, the number of superdiagonals of the matrix A if UPLO = 'U', or the number of subdiagonals if UPLO = 'L'.

Constraint: KD ≥ 0.

4: NRHS – INTEGER *Input*

On entry: r, the number of right-hand sides, i.e., the number of columns of the matrix B.

Constraint: NRHS ≥ 0.

5: AB(LDAB,$*$) – REAL (KIND=nag_wp) array *Input/Output*

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

On entry: the upper or lower triangle of the symmetric band matrix A.

The matrix is stored in rows 1 to $k_d + 1$, more precisely,

if UPLO = 'U', the elements of the upper triangle of A within the band must be stored with element A_{ij} in AB$(k_d + 1 + i - j, j)$ for $\max(1, j - k_d) \leq i \leq j$;

if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element A_{ij} in AB$(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_d)$.

On exit: if INFO $= 0$, the triangular factor U or L from the Cholesky factorization $A = U^{\mathrm{T}}U$ or $A = LL^{\mathrm{T}}$ of the band matrix A, in the same storage format as A.

6: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F07HAF (DPBSV) is called.

Constraint: LDAB $\geq$ KD $+ 1$.

7: B(LDB,$*$) – REAL (KIND=nag_wp) array *Input/Output*

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

On entry: the n by r right-hand side matrix B.

On exit: if INFO $= 0$, the n by r solution matrix X.

8: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07HAF (DPBSV) is called.

Constraint: LDB $\geq \max(1, \mathrm{N})$.

9: INFO – INTEGER *Output*

On exit: INFO $= 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If INFO $= -i$, the ith argument had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, the leading minor of order i of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

7 Accuracy

The computed solution for a single right-hand side, $\hat{x}$, satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the ***machine precision***. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A)\frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = \|A^{-1}\|_1\|A\|_1$, the condition number of A with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) for further details.

F07HBF (DPBSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04BFF solves $Ax = b$ and returns a forward error bound and condition estimate. F04BFF calls F07HAF (DPBSV) to solve the equations.

8 Further Comments

When $n \gg k$, the total number of floating point operations is approximately $n(k+1)^2 + 4nkr$, where k is the number of superdiagonals and r is the number of right-hand sides.

The complex analogue of this routine is F07HNF (ZPBSV).

9 Example

This example solves the equations

$$Ax = b,$$

where A is the symmetric positive definite band matrix

$$A = \begin{pmatrix} 5.49 & 2.68 & 0 & 0 \\ 2.68 & 5.63 & -2.39 & 0 \\ 0 & -2.39 & 2.60 & -2.22 \\ 0 & 0 & -2.22 & 5.17 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 22.09 \\ 9.31 \\ -5.24 \\ 11.83 \end{pmatrix}.$$

Details of the Cholesky factorization of A are also output.

9.1 Program Text

```
    Program f07hafe

!     F07HAF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: dpbsv, nag_wp, x04cef
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter                 :: nin = 5, nout = 6
      Character (1), Parameter           :: uplo = 'U'
!     .. Local Scalars ..
      Integer                            :: i, ifail, info, j, kd, ldab, n
```

```
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: ab(:,:), b(:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max, min
!     .. Executable Statements ..
      Write (nout,*) 'F07HAF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, kd
      ldab = kd + 1
      Allocate (ab(ldab,n),b(n))

!     Read the upper or lower triangular part of the band matrix A
!     from data file

      If (uplo=='U') Then
        Read (nin,*)((ab(kd+1+i-j,j),j=i,min(n,i+kd)),i=1,n)
      Else If (uplo=='L') Then
        Read (nin,*)((ab(1+i-j,j),j=max(1,i-kd),i),i=1,n)
      End If

!     Read b from data file

      Read (nin,*) b(1:n)

!     Solve the equations Ax = b for x
!     The NAG name equivalent of dpbsv is f07haf
      Call dpbsv(uplo,n,kd,1,ab,ldab,b,n,info)

      If (info==0) Then

!       Print solution

        Write (nout,*) 'Solution'
        Write (nout,99999) b(1:n)

!       Print details of factorization

        Write (nout,*)
        Flush (nout)

!       ifail: behaviour on error exit
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        If (uplo=='U') Then
          Call x04cef(n,n,0,kd,ab,ldab,'Cholesky factor U',ifail)
        Else If (uplo=='L') Then
          Call x04cef(n,n,kd,0,ab,ldab,'Cholesky factor L',ifail)
        End If

      Else
        Write (nout,99998) 'The leading minor of order ', info, &
          ' is not positive definite'
      End If

99999 Format ((3X,7F11.4))
99998 Format (1X,A,I3,A)
    End Program f07hafe
```

9.2 Program Data

```
F07HAF Example Program Data

  4      1                 :Values of N and KD

  5.49   2.68
```

```
        5.63  -2.39
              2.60  -2.22
                    5.17 :End of matrix A

22.09   9.31  -5.24  11.83 :End of vector b
```

9.3 Program Results

```
F07HAF Example Program Results

Solution
       5.0000    -2.0000    -3.0000     1.0000

Cholesky factor U
            1          2          3          4
1      2.3431     1.1438
2                 2.0789    -1.1497
3                            1.1306    -1.9635
4                                       1.1465
```