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 Arguments

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 $\geq$ 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, 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, 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, N).

9: INFO – INTEGER *Output*

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

6 Error Indicators and Warnings

INFO < 0

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

INFO > 0

The leading minor of order $\langle value \rangle$ 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 $\kappa(A) = \left\|A^{-1}\right\|_1\|A\|_1$, 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 Parallelism and Performance

F07HAF (DPBSV) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F07HAF (DPBSV) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 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).

10 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.

10.1 Program Text

```
    Program f07hafe

!     F07HAF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. 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
```

10.2 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
```

10.3 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
```