NAG Library Routine Document

F08HAF (DSBEV)

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

F08HAF (DSBEV) computes all the eigenvalues and, optionally, all the eigenvectors of a real n by n symmetric band matrix A of bandwidth $(2k_d + 1)$.

2 Specification

```
SUBROUTINE F08HAF(JOBZ, UPLO, N, KD, AB, LDAB, W, Z, LDZ, WORK, INFO)
INTEGER           N, KD, LDAB, LDZ, INFO
double precision  AB(LDAB,*), W(N), Z(LDZ,*), WORK(3*N-2)
CHARACTER*1       JOBZ, UPLO
```

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

3 Description

The symmetric band matrix A is first reduced to tridiagonal form, using orthogonal similarity transformations, and then the QR algorithm is applied to the tridiagonal matrix to compute the eigenvalues and (optionally) the eigenvectors.

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, Philadelphiahttp://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: JOBZ – CHARACTER*1 *Input*

On entry: if JOBZ = 'N', compute eigenvalues only.

If JOBZ = 'V', compute eigenvalues and eigenvectors.

Constraint: JOBZ = 'N' or 'V'.

2: UPLO – CHARACTER*1 *Input*

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

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

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

3: N – INTEGER *Input*

On entry: the dimension of the array W and n, the order of the matrix A.

Constraint: N $\geq$ 0.

4: KD – INTEGER *Input*

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

If UPLO = 'L', the number of subdiagonals, k_d, of the matrix A.

Constraint: KD ≥ 0.

5: AB(LDAB,$*$) – ***double precision*** 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 n by n 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: AB is overwritten by values generated during the reduction to tridiagonal form.

The first superdiagonal and the diagonal of the tridiagonal matrix T are returned in AB using the same storage format as described above.

6: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F08HAF (DSBEV) is called.

Constraint: LDAB $\geq$ KD + 1.

7: W(N) – ***double precision*** array *Output*

On exit: if INFO = 0, the eigenvalues in ascending order.

8: Z(LDZ,$*$) – ***double precision*** array *Output*

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

On exit: if JOBZ = 'V', then if INFO = 0, Z contains the orthonormal eigenvectors of the matrix A, with the ith column of Z holding the eigenvector associated with W(i).

If JOBZ = 'N', Z is not referenced.

9: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08HAF (DSBEV) is called.

Constraints:

if JOBZ = 'V', LDZ $\geq \max(1, \mathrm{N})$;
otherwise LDZ ≥ 1.

10: WORK($3 \times$ N $- 2$) – ***double precision*** array *Workspace*

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

INFO > 0

If INFO $= i$, the algorithm failed to converge; i off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

7 Accuracy

The computed eigenvalues and eigenvectors are exact for a nearby matrix $(A + E)$, where

$$\|E\|_2 = O(\epsilon)\|A\|_2,$$

and ϵ is the ***machine precision***. See Section 4.7 of Anderson *et al.* (1999) for further details.

8 Further Comments

The total number of floating-point operations is proportional to n^3 if JOBZ = 'V' and is proportional to $k_d n^2$ otherwise.

The complex analogue of this routine is F08HNF (ZHBEV).

9 Example

This example finds all the eigenvalues and eigenvectors of the symmetric band matrix

$$A = \begin{pmatrix} 1 & 2 & 3 & 0 & 0 \\ 2 & 2 & 3 & 4 & 0 \\ 3 & 3 & 3 & 4 & 5 \\ 0 & 4 & 4 & 4 & 5 \\ 0 & 0 & 5 & 5 & 5 \end{pmatrix},$$

together with approximate error bounds for the computed eigenvalues and eigenvectors.

9.1 Program Text

```
*     F08HAF Example Program Text
*     Mark 21 Release.  NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, KDMAX
      PARAMETER        (NMAX=20,KDMAX=5)
      INTEGER          LDAB, LDZ
      PARAMETER        (LDAB=KDMAX+1,LDZ=NMAX)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*     .. Local Scalars ..
      DOUBLE PRECISION EERRBD, EPS
      INTEGER          I, IFAIL, INFO, J, KD, N
*     .. Local Arrays ..
      DOUBLE PRECISION AB(LDAB,NMAX), RCONDZ(NMAX), W(NMAX),
     +                 WORK(3*NMAX-2), Z(LDZ,NMAX), ZERRBD(NMAX)
*     .. External Functions ..
      DOUBLE PRECISION X02AJF
      EXTERNAL         X02AJF
*     .. External Subroutines ..
      EXTERNAL         DDISNA, DSBEV, X04CAF
```

```
*     .. Intrinsic Functions ..
      INTRINSIC        ABS, MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08HAF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD
      IF (N.LE.NMAX .AND. KD.LE.KDMAX) THEN
*
*        Read the upper or lower triangular part of the symmetric band
*        matrix A from data file
*
         IF (UPLO.EQ.'U') THEN
            READ (NIN,*) ((AB(KD+1+I-J,J),J=I,MIN(N,I+KD)),I=1,N)
         ELSE IF (UPLO.EQ.'L') THEN
            READ (NIN,*) ((AB(1+I-J,J),J=MAX(1,I-KD),I),I=1,N)
         END IF
*
*        Solve the band symmetric eigenvalue problem
*
         CALL DSBEV('Vectors',UPLO,N,KD,AB,LDAB,W,Z,LDZ,WORK,INFO)
*
         IF (INFO.EQ.0) THEN
*
*           Print solution
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (W(J),J=1,N)
*
            IFAIL = 0
            CALL X04CAF('General',' ',N,N,Z,LDZ,'Eigenvectors',IFAIL)
*
*           Get the machine precision, EPS and compute the approximate
*           error bound for the computed eigenvalues.  Note that for
*           the 2-norm, max( abs(W(i)) ) = norm(A), and since the
*           eigenvalues are returned in ascending order
*           max( abs(W(i)) ) = max( abs(W(1)), abs(W(n)))
*
            EPS = X02AJF()
            EERRBD = EPS*MAX(ABS(W(1)),ABS(W(N)))
*
*           Call DDISNA (F08FLF) to estimate reciprocal condition
*           numbers for the eigenvectors
*
            CALL DDISNA('Eigenvectors',N,N,W,RCONDZ,INFO)
*
*           Compute the error estimates for the eigenvectors
*
            DO 20 I = 1, N
               ZERRBD(I) = EERRBD/RCONDZ(I)
   20       CONTINUE
*
*           Print the approximate error bounds for the eigenvalues
*           and vectors
*
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Error estimate for the eigenvalues'
            WRITE (NOUT,99998) EERRBD
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Error estimates for the eigenvectors'
            WRITE (NOUT,99998) (ZERRBD(I),I=1,N)
         ELSE
            WRITE (NOUT,99997) 'Failure in DSBEV. INFO =', INFO
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX and/or KDMAX too small'
      END IF
```

```
*
99999 FORMAT (3X,(8F8.4))
99998 FORMAT (4X,1P,6E11.1)
99997 FORMAT (1X,A,I4)
      END
```

9.2 Program Data

```
F08HAF Example Program Data

  5    2                   :Values of N and KD

  1.0  2.0  3.0
       2.0  3.0  4.0
            3.0  4.0  5.0
                 4.0  5.0
                      5.0  :End of matrix A
```

9.3 Program Results

```
 F08HAF Example Program Results

 Eigenvalues
    -3.2474 -2.6633  1.7511  4.1599 14.9997
 Eigenvectors
          1       2       3       4       5
 1   0.0394  0.6238  0.5635 -0.5165  0.1582
 2   0.5721 -0.2575 -0.3896 -0.5955  0.3161
 3  -0.4372 -0.5900  0.4008 -0.1470  0.5277
 4  -0.4424  0.4308 -0.5581  0.0470  0.5523
 5   0.5332  0.1039  0.2421  0.5956  0.5400

 Error estimate for the eigenvalues
        1.7E-15

 Error estimates for the eigenvectors
        2.9E-15    2.9E-15    6.9E-16    6.9E-16    1.5E-16
```