NAG Library Routine Document

F08HCF (DSBEVD)

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.

Warning. The specification of the parameters LWORK and LIWORK changed at Mark 20 in the case where JOB = 'V' and N > 1: the minimum dimension of the array WORK has been reduced whereas the minimum dimension of the array IWORK has been increased.

1 Purpose

F08HCF (DSBEVD) computes all the eigenvalues and, optionally, all the eigenvectors of a real symmetric band matrix. If the eigenvectors are requested, then it uses a divide-and-conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal–Walker–Kahan variant of the QL or QR algorithm.

2 Specification

```
 SUBROUTINE F08HCF(JOB, UPLO, N, KD, AB, LDAB, W, Z, LDZ, WORK, LWORK,
1                  IWORK, LIWORK, INFO)
 INTEGER           N, KD, LDAB, LDZ, LWORK, IWORK(max(1,LIWORK)), LIWORK,
1                  INFO
 double precision  AB(LDAB,*), W(*), Z(LDZ,*), WORK(max(1,LWORK))
 CHARACTER*1       JOB, UPLO
```

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

3 Description

F08HCF (DSBEVD) computes all the eigenvalues and, optionally, all the eigenvectors of a real symmetric band matrix A. In other words, it can compute the spectral factorization of A as

$$A = Z\Lambda Z^{\mathrm{T}},$$

where Λ is a diagonal matrix whose diagonal elements are the eigenvalues λ_i, and Z is the orthogonal matrix whose columns are the eigenvectors z_i. Thus

$$Az_i = \lambda_i z_i, \qquad i = 1, 2, \ldots, n.$$

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: JOB – CHARACTER*1 *Input*

On entry: indicates whether eigenvectors are computed.

JOB = 'N'
Only eigenvalues are computed.

JOB = 'V'
Eigenvalues and eigenvectors are computed.

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

2: UPLO – CHARACTER*1 *Input*

On entry: indicates whether the upper or lower triangular part of A is stored.

UPLO = 'U'
The upper triangular part of A is stored.

UPLO = 'L'
The lower triangular part of A is stored.

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

3: N – INTEGER *Input*

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

Constraint: N ≥ 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 $\mathrm{AB}(k_d + 1 + i - j, j)$ 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 $\mathrm{AB}(1 + i - j, j)$ 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 F08HCF (DSBEVD) is called.

Constraint: LDAB $\geq$ KD + 1.

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

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

On exit: the eigenvalues of the matrix A in ascending order.

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

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

On exit: if JOB = 'V', Z is overwritten by the orthogonal matrix Z which contains the eigenvectors of A. The ith column of Z contains the eigenvector which corresponds to the eigenvalue $\mathrm{W}(i)$.

If JOB = '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 F08HCF (DSBEVD) is called.

Constraints:

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

10: WORK$(\max(1, \mathrm{LWORK}))$ – ***double precision*** array *Workspace*

On exit: if INFO $= 0$, WORK(1) contains the required minimal size of LWORK.

11: LWORK – INTEGER *Input*

On entry: the dimension of the array WORK as declared in the (sub)program from which F08HCF (DSBEVD) is called.

If LWORK $= -1$, a workspace query is assumed; the routine only calculates the minimum dimension of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

Constraints:

if $\mathrm{N} \leq 1$, LWORK ≥ 1 or LWORK $= -1$;
if JOB = 'N' and $\mathrm{N} > 1$, LWORK $\geq 2 \times \mathrm{N}$ or LWORK $= -1$;
if JOB = 'V' and $\mathrm{N} > 1$, LWORK $\geq 2 \times \mathrm{N}^2 + 5 \times \mathrm{N} + 1$ or LWORK $= -1$.

12: IWORK$(\max(1, \mathrm{LIWORK}))$ – INTEGER array *Workspace*

On exit: if INFO $= 0$, IWORK(1) contains the required minimal size of LIWORK.

13: LIWORK – INTEGER *Input*

On entry: the dimension of the array IWORK as declared in the (sub)program from which F08HCF (DSBEVD) is called.

If LIWORK $= -1$, a workspace query is assumed; the routine only calculates the minimum dimension of the IWORK array, returns this value as the first entry of the IWORK array, and no error message related to LIWORK is issued.

Constraints:

if JOB = 'N' or $\mathrm{N} \leq 1$, LIWORK ≥ 1 or LIWORK $= -1$;
if JOB = 'V' and $\mathrm{N} > 1$, LIWORK $\geq 5 \times \mathrm{N} + 3$ or LIWORK $= -1$.

14: 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 $= i$ and JOB = 'N', the algorithm failed to converge; i elements of an intermediate tridiagonal form did not converge to zero; if INFO $= i$ and JOB = 'V', then the algorithm failed to

compute an eigenvalue while working on the submatrix lying in rows and column $i/(\mathrm{N}+1)$ through $\mathrm{mod}(i, \mathrm{N}+1)$.

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 complex analogue of this routine is F08HQF (ZHBEVD).

9 Example

This example computes all the eigenvalues and eigenvectors of the symmetric band matrix A, where

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

9.1 Program Text

```
*     F08HCF Example Program Text
*     Mark 20 Revised. NAG Copyright 2001.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, KDMAX, LDAB, LDZ
      PARAMETER        (NMAX=9,KDMAX=4,LDAB=KDMAX,LDZ=NMAX)
      INTEGER          LWORK, LIWORK
      PARAMETER        (LWORK=2*NMAX*NMAX+5*NMAX+1,LIWORK=5*NMAX+3)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, KD, N
      CHARACTER        JOB, UPLO
*     .. Local Arrays ..
      DOUBLE PRECISION AB(LDAB,NMAX), W(NMAX), WORK(LWORK), Z(LDZ,NMAX)
      INTEGER          IWORK(LIWORK)
*     .. External Subroutines ..
      EXTERNAL         DSBEVD, X04CAF
*     .. Intrinsic Functions ..
      INTRINSIC        MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08HCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD
      IF (N.LE.NMAX) THEN
*
*        Read A from data file
*
         READ (NIN,*) UPLO
         IF (UPLO.EQ.'U') THEN
            DO 20 I = 1, N
               READ (NIN,*) (AB(KD+1+I-J,J),J=I,MIN(N,I+KD))
   20       CONTINUE
         ELSE IF (UPLO.EQ.'L') THEN
            DO 40 I = 1, N
               READ (NIN,*) (AB(1+I-J,J),J=MAX(1,I-KD),I)
   40       CONTINUE
         END IF
*
         READ (NIN,*) JOB
```

```
*
*        Calculate all the eigenvalues and eigenvectors of A
*
         CALL DSBEVD(JOB,UPLO,N,KD,AB,LDAB,W,Z,LDZ,WORK,LWORK,IWORK,
     +              LIWORK,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.GT.0) THEN
            WRITE (NOUT,*) 'Failure to converge.'
         ELSE
*
*           Print eigenvalues and eigenvectors
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (W(I),I=1,N)
            WRITE (NOUT,*)
            IFAIL = 0
*
            CALL X04CAF('General',' ',N,N,Z,LDZ,'Eigenvectors',IFAIL)
*
         END IF
      END IF
*
99999 FORMAT (3X,(8F8.4))
      END
```

9.2 Program Data

```
F08HCF Example Program Data
  5  2                       :Values of N and KD
  'L'                        :Value of UPLO
  1.0
  2.0  2.0
  3.0  3.0  3.0
       4.0  4.0  4.0
            5.0  5.0  5.0    :End of matrix A
  'V'                        :Value of JOB
```

9.3 Program Results

```
 F08HCF 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
```