NAG Fortran Library Routine Document

F08HNF (ZHBEV)

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

F08HNF (ZHBEV) computes all the eigenvalues and, optionally, eigenvectors of a complex n by n Hermitian band matrix A of bandwidth $(2k_d + 1)$.

2 Specification

```
      SUBROUTINE F08HNF (JOBZ, UPLO, N, KD, AB, LDAB, W, Z, LDZ, WORK, RWORK,
     1                   INFO)
      INTEGER            N, KD, LDAB, LDZ, INFO
      double precision   W(*), RWORK(*)
      complex*16         AB(LDAB,*), Z(LDZ,*), WORK(*)
      CHARACTER*1        JOBZ, UPLO
```

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

3 Description

The Hermitian band matrix A is first reduced to real tridiagonal form, using unitary 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, Philadelphia URL: 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: 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 triangle of A is stored.

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

3: N – INTEGER *Input*

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

Constraint: N ≥ 0.

4: KD – INTEGER *Input*

On entry: k_d, the number of super-diagonals of the matrix A if UPLO = 'U', or the number of sub-diagonals if UPLO = 'L'.

Constraint: KD ≥ 0.

5: AB(LDAB,$*$) – ***complex*16*** 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 Hermitian band matrix A, stored in the first KD $+ 1$ rows of the array. The jth column of A is stored in the jth column of the array AB as follows:

if UPLO = 'U', $\mathrm{AB}(k_d + 1 + i - j, j) = a_{ij}$ for $\max(1, j - k_d) \leq i \leq j$;
if UPLO = 'L', $\mathrm{AB}(1 + i - j, j) = a_{ij}$ for $j \leq i \leq \min(n, j + k_d)$.

On exit: is overwritten by values generated during the reduction to tridiagonal form. If UPLO = 'U' , the first super-diagonal and the diagonal of the tridiagonal matrix T are returned in rows KD and KD $+ 1$ of AB, and if UPLO = 'L', the diagonal and first sub-diagonal of T are returned in the first two rows of AB.

6: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F08HNF (ZHBEV) 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: if INFO = 0, the eigenvalues in ascending order.

8: Z(LDZ,$*$) – ***complex*16*** 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 F08HNF (ZHBEV) is called.

Constraints:

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

10: WORK($*$) – ***complex*16*** array *Workspace*

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

11: RWORK($*$) – ***double precision*** array *Workspace*

Note: the dimension of the array RWORK must be at least $\max(1, 3 \times \mathrm{N} - 2)$.

12: 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.

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

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

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 real analogue of this routine is F08HAF (DSBEV).

9 Example

To find all the eigenvalues and eigenvectors of the Hermitian band matrix

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

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

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.

```
*     F08HNF Example Program Text
*     Mark 21.  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 ..
      COMPLEX *16      AB(LDAB,NMAX), WORK(NMAX), Z(LDZ,NMAX)
      DOUBLE PRECISION RCONDZ(NMAX), RWORK(3*NMAX-2), W(NMAX),
     +                 ZERRBD(NMAX)
*     .. External Functions ..
```

```
      DOUBLE PRECISION X02AJF
      EXTERNAL         X02AJF
*     .. External Subroutines ..
      EXTERNAL         DDISNA, X04DAF, ZHBEV
*     .. Intrinsic Functions ..
      INTRINSIC        ABS, MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08HNF 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 Hermitian eigenvalue problem
*
         CALL ZHBEV('Vectors',UPLO,N,KD,AB,LDAB,W,Z,LDZ,WORK,RWORK,INFO)
*
         IF (INFO.EQ.0) THEN
*
*           Print solution
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (W(J),J=1,N)
*
            IFAIL = 0
            CALL X04DAF('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 ZHBEV. INFO =', INFO
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX and/or KDMAX too small'
```

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

9.2 Program Data

```
F08HNF Example Program Data

   5         2                                          :Values of N and KD

  (1.0, 0.0) (2.0,-1.0) (3.0,-1.0)
             (2.0, 0.0) (3.0,-2.0) (4.0,-2.0)
                        (3.0, 0.0) (4.0,-3.0) (5.0,-3.0)
                                   (4.0, 0.0) (5.0,-4.0)
                                              (5.0, 0.0) :End of matrix A
```

9.3 Program Results

```
 F08HNF Example Program Results

 Eigenvalues
    -6.4185 -1.4094  1.4421  4.4856 16.9002
 Eigenvectors
          1       2       3       4       5
 1  -0.2534  0.6367 -0.2560  0.0171  0.1051
    -0.0538  0.0000  0.3721  0.5500 -0.0983

 2  -0.0662 -0.2578  0.5344 -0.2608  0.2516
     0.4301  0.2413  0.0000  0.4869 -0.1789

 3   0.5274 -0.3039 -0.4245 -0.0399  0.4994
     0.0000 -0.3481  0.0915  0.2142 -0.1513

 4   0.1061  0.3450  0.4964 -0.0253  0.5611
    -0.4981 -0.0832 -0.1546 -0.1700  0.0000

 5  -0.4519 -0.2469 -0.1979  0.5614  0.4837
     0.0424  0.2634 -0.1114  0.0000  0.2509

 Error estimate for the eigenvalues
        1.9E-15

 Error estimates for the eigenvectors
        3.7E-16    6.6E-16    6.6E-16    6.2E-16    1.5E-16
```