NAG Library Routine Document

F08HPF (ZHBEVX)

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

F08HPF (ZHBEVX) computes selected eigenvalues and, optionally, eigenvectors of a complex n by n Hermitian band matrix A of bandwidth $(2k_d + 1)$. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Specification

```
SUBROUTINE F08HPF (JOBZ, RANGE, UPLO, N, KD, AB, LDAB, Q, LDQ, VL, VU, IL,      &
                   IU, ABSTOL, M, W, Z, LDZ, WORK, RWORK, IWORK, JFAIL,         &
                   INFO)

INTEGER               N, KD, LDAB, LDQ, IL, IU, M, LDZ, IWORK(5*N),             &
                      JFAIL(*), INFO
REAL (KIND=nag_wp)    VL, VU, ABSTOL, W(N), RWORK(7*N)
COMPLEX (KIND=nag_wp) AB(LDAB,*), Q(LDQ,*), Z(LDZ,*), WORK(N)
CHARACTER(1)          JOBZ, RANGE, UPLO
```

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

3 Description

The Hermitian band matrix A is first reduced to real tridiagonal form, using unitary similarity transformations. The required eigenvalues and eigenvectors are then computed from the tridiagonal matrix; the method used depends upon whether all, or selected, eigenvalues and eigenvectors are required.

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

Demmel J W and Kahan W (1990) Accurate singular values of bidiagonal matrices *SIAM J. Sci. Statist. Comput.* **11** 873–912

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: indicates whether eigenvectors are computed.

JOBZ = 'N'
Only eigenvalues are computed.

JOBZ = 'V'
Eigenvalues and eigenvectors are computed.

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

2: RANGE – CHARACTER(1) *Input*

On entry: if RANGE = 'A', all eigenvalues will be found.

If RANGE = 'V', all eigenvalues in the half-open interval $(\mathrm{VL}, \mathrm{VU}]$ will be found.

If RANGE = 'I', the ILth to IUth eigenvalues will be found.

Constraint: RANGE = 'A', 'V' or 'I'.

3: 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'.

4: N – INTEGER *Input*

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

Constraint: $\mathrm{N} \geq 0$.

5: 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: $\mathrm{KD} \geq 0$.

6: AB(LDAB,$*$) – COMPLEX (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 n by n Hermitian 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 or subdiagonal and the diagonal of the tridiagonal matrix T are returned in AB using the same storage format as described above.

7: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F08HPF (ZHBEVX) is called.

Constraint: $\mathrm{LDAB} \geq \mathrm{KD} + 1$.

8: Q(LDQ,$*$) – COMPLEX (KIND=nag_wp) array *Output*

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

On exit: if JOBZ = 'V', the n by n unitary matrix used in the reduction to tridiagonal form.

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

9: LDQ – INTEGER *Input*

On entry: the first dimension of the array Q as declared in the (sub)program from which F08HPF (ZHBEVX) is called.

Constraints:

if JOBZ = 'V', LDQ $\geq \max(1, N)$;
otherwise LDQ ≥ 1.

10: VL – REAL (KIND=nag_wp) *Input*
11: VU – REAL (KIND=nag_wp) *Input*

On entry: if RANGE = 'V', the lower and upper bounds of the interval to be searched for eigenvalues.

If RANGE = 'A' or 'I', VL and VU are not referenced.

Constraint: if RANGE = 'V', VL < VU.

12: IL – INTEGER *Input*
13: IU – INTEGER *Input*

On entry: if RANGE = 'I', the indices (in ascending order) of the smallest and largest eigenvalues to be returned.

If RANGE = 'A' or 'V', IL and IU are not referenced.

Constraints:

if RANGE = 'I' and N = 0, IL = 1 and IU = 0;
if RANGE = 'I' and N > 0, $1 \leq \mathrm{IL} \leq \mathrm{IU} \leq \mathrm{N}$.

14: ABSTOL – REAL (KIND=nag_wp) *Input*

On entry: the absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a, b]$ of width less than or equal to

$$\mathrm{ABSTOL} + \epsilon \max(|a|, |b|),$$

where ϵ is the ***machine precision***. If ABSTOL is less than or equal to zero, then $\epsilon \|T\|_1$ will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when ABSTOL is set to twice the underflow threshold $2 \times$ X02AMF( ), not zero. If this routine returns with INFO > 0, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times$ X02AMF( ). See Demmel and Kahan (1990).

15: M – INTEGER *Output*

On exit: the total number of eigenvalues found. $0 \leq \mathrm{M} \leq \mathrm{N}$.

If RANGE = 'A', M = N.

If RANGE = 'I', M = IU − IL + 1.

16: W(N) – REAL (KIND=nag_wp) array *Output*

On exit: the first M elements contain the selected eigenvalues in ascending order.

17: Z(LDZ,$*$) – COMPLEX (KIND=nag_wp) array *Output*

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

On exit: if JOBZ = 'V', then

if INFO = 0, the first M columns of Z contain the orthonormal eigenvectors of the matrix A corresponding to the selected eigenvalues, with the ith column of Z holding the eigenvector associated with W(i);

if an eigenvector fails to converge (INFO > 0), then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in JFAIL.

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

Note: you must ensure that at least $\max(1, M)$ columns are supplied in the array Z; if RANGE = 'V', the exact value of M is not known in advance and an upper bound of at least N must be used.

18: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08HPF (ZHBEVX) is called.

Constraints:

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

19: WORK(N) – COMPLEX (KIND=nag_wp) array *Workspace*

20: RWORK($7 \times N$) – REAL (KIND=nag_wp) array *Workspace*

21: IWORK($5 \times N$) – INTEGER array *Workspace*

22: JFAIL($*$) – INTEGER array *Output*

Note: the dimension of the array JFAIL must be at least $\max(1, N)$.

On exit: if JOBZ = 'V', then

if INFO = 0, the first M elements of JFAIL are zero;

if INFO > 0, JFAIL contains the indices of the eigenvectors that failed to converge.

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

23: 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 $= i$, then i eigenvectors failed to converge. Their indices are stored in array JFAIL. Please see ABSTOL.

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 $k_d n^2$ if JOBZ = 'N', and is proportional to n^3 if JOBZ = 'V' and RANGE = 'A', otherwise the number of floating point operations will depend upon the number of computed eigenvectors.

The real analogue of this routine is F08HBF (DSBEVX).

9 Example

This example finds the eigenvalues in the half-open interval $(-2, 2]$, and the corresponding eigenvectors, of the Hermitian band matrix

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

9.1 Program Text

```
    Program f08hpfe

!     F08HPF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, x04daf, zhbevx
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Real (Kind=nag_wp), Parameter    :: zero = 0.0E+0_nag_wp
      Integer, Parameter               :: nin = 5, nout = 6
      Character (1), Parameter         :: uplo = 'U'
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: abstol, vl, vu
      Integer                          :: i, ifail, il, info, iu, j, kd, ldab, &
                                          ldq, ldz, m, n
!     .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: ab(:,:), q(:,:), work(:), z(:,:)
      Real (Kind=nag_wp), Allocatable  :: rwork(:), w(:)
      Integer, Allocatable             :: iwork(:), jfail(:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max, min
!     .. Executable Statements ..
      Write (nout,*) 'F08HPF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, kd
      ldab = kd + 1
      ldq = n
      ldz = n
      m = n
      Allocate (ab(ldab,n),q(ldq,n),work(n),z(ldz,m),rwork(7*n),w(n), &
        iwork(5*n),jfail(n))

!     Read the lower and upper bounds of the interval to be searched,
!     and read the upper or lower triangular part of the matrix A
!     from data file

      Read (nin,*) vl, vu
      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

!     Set the absolute error tolerance for eigenvalues.  With ABSTOL
!     set to zero, the default value is used instead

      abstol = zero

!     Solve the band symmetric eigenvalue problem
!     The NAG name equivalent of zhbevx is f08hpf
```

```
      Call zhbevx('Vectors','Values in range',uplo,n,kd,ab,ldab,q,ldq,vl,vu, &
        il,iu,abstol,m,w,z,ldz,work,rwork,iwork,jfail,info)

      If (info>=0) Then

!       Print solution

        Write (nout,99999) 'Number of eigenvalues found =', m
        Write (nout,*)
        Write (nout,*) 'Eigenvalues'
        Write (nout,99998) w(1:m)
        Flush (nout)

!       ifail: behaviour on error exit
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        Call x04daf('General',' ',n,m,z,ldz,'Selected eigenvectors',ifail)

        If (info>0) Then
          Write (nout,99999) 'INFO eigenvectors failed to converge, INFO =', &
            info
          Write (nout,*) 'Indices of eigenvectors that did not converge'
          Write (nout,99997) jfail(1:m)
        End If
      Else
        Write (nout,99999) 'Failure in ZHBEVX. INFO =', info
      End If

99999 Format (1X,A,I5)
99998 Format (3X,(8F8.4))
99997 Format (3X,(8I8))
    End Program f08hpfe
```

9.2 Program Data

```
F08HPF Example Program Data

   5          2                                         :Values of N and KD

  -2.0        2.0                                       :Values of VL and VU

  (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

```
 F08HPF Example Program Results

 Number of eigenvalues found =    2

 Eigenvalues
   -1.4094  1.4421
 Selected eigenvectors
          1       2
 1   0.6367  0.4516
     0.0000  0.0000

 2  -0.2578 -0.3029
     0.2413 -0.4402

 3  -0.3039  0.3160
    -0.3481  0.2978
```

```
 4   0.3450 -0.4088
    -0.0832 -0.3213

 5  -0.2469  0.0204
     0.2634  0.2262
```