NAG Toolbox

nag_lapack_zhbevx (f08hp)

1 Purpose

nag_lapack_zhbevx (f08hp) 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 Syntax

```
[ab, q, m, w, z, jfail, info] = nag_lapack_zhbevx(jobz, range, uplo, kd, ab, vl, vu, il, iu, abstol, 'n', n)
[ab, q, m, w, z, jfail, info] = f08hp(jobz, range, uplo, kd, ab, vl, vu, il, iu, abstol, 'n', n)
```

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

5.1 Compulsory Input Parameters

1: **jobz** – CHARACTER(1)

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)

If **range** = 'A', all eigenvalues will be found.

If **range** = 'V', all eigenvalues in the half-open interval $(\mathbf{vl}, \mathbf{vu}]$ will be found.

If **range** = 'I', the **il**th to **iu**th eigenvalues will be found.

Constraint: **range** = 'A', 'V' or 'I'.

3: **uplo** – CHARACTER(1)

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: **kd** – INTEGER

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**$(ldab,:)$ – COMPLEX (KIND=nag_wp) array

The first dimension of the array **ab** must be at least **kd** $+ 1$.

The second dimension of the array **ab** must be at least $\max(1, \mathbf{n})$.

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 **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 $j \leq i \leq \min(n, j + k_d)$.

6: **vl** – REAL (KIND=nag_wp)

7: **vu** – REAL (KIND=nag_wp)

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**.

8: **il** – INTEGER

9: **iu** – INTEGER

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, $1 \leq$ **il** $\leq$ **iu** $\leq$ **n**.

10: **abstol** – REAL (KIND=nag_wp)

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

$$\mathbf{abstol} + \epsilon \max(|a|, |b|),$$

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 $2 \times$ x02am( ), not zero. If this function returns with **info** > 0, indicating that some

eigenvectors did not converge, try setting **abstol** to $2 \times$ x02am( ). See Demmel and Kahan (1990).

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the second dimension of the array **ab**.

n, the order of the matrix A.

Constraint: $\mathbf{n} \geq 0$.

5.3 Output Parameters

1: **ab**$(ldab, :)$ – COMPLEX (KIND=nag_wp) array

The first dimension of the array **ab** will be $\mathbf{kd} + 1$.

The second dimension of the array **ab** will be $\max(1, \mathbf{n})$.

ab stores 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.

2: **q**$(ldq, :)$ – COMPLEX (KIND=nag_wp) array

The first dimension, ldq, of the array **q** will be

if **jobz** = 'V', $ldq = \max(1, \mathbf{n})$;
otherwise $ldq = 1$.

The second dimension of the array **q** will be $\max(1, \mathbf{n})$ if **jobz** = 'V' and 1 otherwise.

If **jobz** = 'V', the n by n unitary matrix used in the reduction to tridiagonal form.

If **jobz** = 'N', **q** is not referenced.

3: **m** – INTEGER

The total number of eigenvalues found. $0 \leq \mathbf{m} \leq \mathbf{n}$.

If **range** = 'A', $\mathbf{m} = \mathbf{n}$.

If **range** = 'I', $\mathbf{m} = \mathbf{iu} - \mathbf{il} + 1$.

4: **w**$(\mathbf{n})$ – REAL (KIND=nag_wp) array

The first **m** elements contain the selected eigenvalues in ascending order.

5: **z**$(ldz, :)$ – COMPLEX (KIND=nag_wp) array

The first dimension, ldz, of the array **z** will be

if **jobz** = 'V', $ldz = \max(1, \mathbf{n})$;
otherwise $ldz = 1$.

The second dimension of the array **z** will be $\max(1, \mathbf{m})$ if **jobz** = 'V' and 1 otherwise.

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.

6: **jfail**(:) – INTEGER array

The dimension of the array **jfail** will be $\max(1, \mathbf{n})$

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.

7: **info** – INTEGER

info $= 0$ unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

info $= -i$

If **info** $= -i$, parameter i had an illegal value on entry. The parameters are numbered as follows:

1: **jobz**, 2: **range**, 3: **uplo**, 4: **n**, 5: **kd**, 6: **ab**, 7: **ldab**, 8: **q**, 9: **ldq**, 10: **vl**, 11: **vu**, 12: **il**, 13: **iu**, 14: **abstol**, 15: **m**, 16: **w**, 17: **z**, 18: **ldz**, 19: **work**, 20: **rwork**, 21: **iwork**, 22: **jfail**, 23: **info**.

It is possible that **info** refers to a parameter that is omitted from the MATLAB interface. This usually indicates that an error in one of the other input parameters has caused an incorrect value to be inferred.

info > 0 (*warning*)

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 function is nag_lapack_dsbevx (f08hb).

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

```
     function f08hp_example

fprintf('f08hp example results\n\n');

% Hermitian band matrix A, stored on symmetric banded format
uplo = 'U';
kd   = nag_int(2);
ab = [0,       0 + 0i,  3 - 1i,  4 - 2i,  5 - 3i;
      0 + 0i,  2 - 1i,  3 - 2i,  4 - 3i,  5 - 4i;
      1 + 0i,  2 + 0i,  3 + 0i,  4 + 0i,  5 + 0i];

% Eigenvalues in range [-2,2] and coresponding eigenvectors
jobz = 'Vectors';
range = 'Values in range';
vl = -2;
vu = 2;
il = nag_int(0);
iu = nag_int(0);
abstol = 0;
[~, q, m, w, z, jfail, info] = ...
f08hp( ...
       jobz, range, uplo, kd, ab, vl, vu, il, iu, abstol);

% Normalize: largest elements are real
for i = 1:m
  [~,k] = max(abs(real(z(:,i)))+abs(imag(z(:,i))));
  z(:,i) = z(:,i)*conj(z(k,i))/abs(z(k,i));
end

disp('Eigenvalues in range [-2,2]');
disp(w(1:m)');
[ifail] = x04da( ...
                 'General', ' ', z, 'Corresponding eigenvectors');
```

9.2 Program Results

```
     f08hp example results

Eigenvalues in range [-2,2]
   -1.4094    1.4421

 Corresponding eigenvectors
          1       2
 1  -0.4188 -0.2560
     0.4797  0.3721

 2  -0.0122  0.5344
    -0.3529  0.0000

 3   0.4621 -0.4245
     0.0000  0.0915

 4  -0.1642  0.4964
     0.3146 -0.1546

 5  -0.0360 -0.1979
    -0.3593 -0.1114
```