NAG Toolbox

nag_lapack_zheevx (f08fp)

1 Purpose

nag_lapack_zheevx (f08fp) computes selected eigenvalues and, optionally, eigenvectors of a complex n by n Hermitian matrix A. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Syntax

```
[a, m, w, z, jfail, info] = nag_lapack_zheevx(jobz, range, uplo, a, vl, vu, il,
iu, abstol, 'n', n)
```

```
[a, m, w, z, jfail, info] = f08fp(jobz, range, uplo, a, vl, vu, il, iu, abstol,
'n', n)
```

3 Description

The Hermitian 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: **a**$(lda,:)$ – COMPLEX (KIND=nag_wp) array

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

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

The n by n Hermitian matrix A.

If **uplo** = 'U', the upper triangular part of a must be stored and the elements of the array below the diagonal are not referenced.

If **uplo** = 'L', the lower triangular part of a must be stored and the elements of the array above the diagonal are not referenced.

5: **vl** – REAL (KIND=nag_wp)
6: **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', $\mathbf{vl} < \mathbf{vu}$.

7: **il** – INTEGER
8: **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 $\mathbf{n} = 0$, $\mathbf{il} = 1$ and $\mathbf{iu} = 0$;
if **range** = 'I' and $\mathbf{n} > 0$, $1 \leq \mathbf{il} \leq \mathbf{iu} \leq \mathbf{n}$.

9: **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 $\mathbf{info} > 0$, 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 first dimension of the array **a** and the second dimension of the array **a**. (An error is raised if these dimensions are not equal.)

n, the order of the matrix A.

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

5.3 Output Parameters

1: **a**$(lda,:)$ – COMPLEX (KIND=nag_wp) array

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

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

The lower triangle (if **uplo** = 'L') or the upper triangle (if **uplo** = 'U') of **a**, including the diagonal, is overwritten.

2: **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', $\mathbf{m} = \mathbf{iu} - \mathbf{il} + 1$.

3: **w**$(:)$ – REAL (KIND=nag_wp) array

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

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

4: **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 $\mathbf{w}(i)$;

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.

5: **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.

6: **info** – INTEGER

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

6 Error Indicators and Warnings

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 (*warning*)

The algorithm failed to converge; $\langle$*value*$\rangle$ eigenvectors did not converge. Their indices are stored in array **jfail**.

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.

The real analogue of this function is nag_lapack_dsyevx (f08fb).

9 Example

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

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

9.1 Program Text

```
function f08fp_example

fprintf('f08fp example results\n\n');

% Eigenvalues between -2 and 2 of A, and corresponding eigenvectors.
a = [ 1 + 0i,  2 - 1i,  3 - 1i,  4 - 1i;
      0 + 0i,  2 + 0i,  3 - 2i,  4 - 2i;
      0 + 0i,  0 + 0i,  3 + 0i,  4 - 3i;
      0 + 0i,  0 + 0i,  0 + 0i,  4 + 0i];

jobz  = 'Vectors';
range = 'Values in range';
uplo  = 'Upper';
vl = -2;
vu =  2;
il = nag_int(0);
iu = nag_int(0);
abstol = 0;
[~, m, w, z, jfail, info] = ...
  f08fp(...
        jobz, range, uplo, a, vl, vu, il, iu, abstol);

% Normalize
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
```

```
fprintf('Number of eigenvalues in [-2,2] is %2d\n',m);
fprintf('\n Eigenvalues are:\n');
disp(w(1:m));

ncols  = nag_int(80);
indent = nag_int(0);
[ifail] = x04db( ...
                 'General', ' ', z, 'Bracketed', 'F7.4', ...
                 'Corresponding eigenvectors', 'Integer', 'Integer', ...
                 ncols, indent);
```

9.2 Program Results

```
     f08fp example results

Number of eigenvalues in [-2,2] is  2

 Eigenvalues are:
   -0.6886
    1.1412

 Corresponding eigenvectors
                   1                  2
 1  ( 0.6470, 0.0000) ( 0.0179,-0.4453)
 2  (-0.4984,-0.1130) ( 0.5706, 0.0000)
 3  ( 0.2949, 0.3165) (-0.1530, 0.5273)
 4  (-0.2241,-0.2878) (-0.2118,-0.3598)
```