NAG Toolbox

nag_lapack_zheevd (f08fq)

1 Purpose

nag_lapack_zheevd (f08fq) computes all the eigenvalues and, optionally, all the eigenvectors of a complex Hermitian 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 Syntax

```
[a, w, info] = nag_lapack_zheevd(job, uplo, a, 'n', n)
[a, w, info] = f08fq(job, uplo, a, 'n', n)
```

3 Description

nag_lapack_zheevd (f08fq) computes all the eigenvalues and, optionally, all the eigenvectors of a complex Hermitian matrix A. In other words, it can compute the spectral factorization of A as

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

where Λ is a real diagonal matrix whose diagonal elements are the eigenvalues λ_i, and Z is the (complex) unitary matrix whose columns are the eigenvectors z_i. Thus

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

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, Philadelphia 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

5.1 Compulsory Input Parameters

1: **job** – CHARACTER(1)

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)

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: **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.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the array **a** and the second dimension of the array **a**.

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 $\max(1,\mathbf{n})$.

If **job** = 'V', **a** stores the unitary matrix Z which contains the eigenvectors of A.

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

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

The eigenvalues of the matrix A in ascending order.

3: **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: **job**, 2: **uplo**, 3: **n**, 4: **a**, 5: **lda**, 6: **w**, 7: **work**, 8: **lwork**, 9: **rwork**, 10: **lrwork**, 11: **iwork**, 12: **liwork**, 13: **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

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 $i/(\mathbf{n}+1)$ through i mod $(\mathbf{n}+1)$.

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 real analogue of this function is nag_lapack_dsyevd (f08fc).

9 Example

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

$$A = \begin{pmatrix} 1.0+0.0i & 2.0-1.0i & 3.0-1.0i & 4.0-1.0i \\ 2.0+1.0i & 2.0+0.0i & 3.0-2.0i & 4.0-2.0i \\ 3.0+1.0i & 3.0+2.0i & 3.0+0.0i & 4.0-3.0i \\ 4.0+1.0i & 4.0+2.0i & 4.0+3.0i & 4.0+0.0i \end{pmatrix}.$$

The example program for nag_lapack_zheevd (f08fq) illustrates the computation of error bounds for the eigenvalues and eigenvectors.

9.1 Program Text

```
function f08fq_example

fprintf('f08fq example results\n\n');

% Lower triangular part of Hermitian matrix A
uplo = 'L';
n = 4;
a = [ 1 + 0i,  0 + 0i,  0 + 0i,  0 + 0i;
      2 + 1i,  2 + 0i,  0 + 0i,  0 + 0i;
      3 + 1i,  3 + 2i,  3 + 0i,  0 + 0i;
      4 + 1i,  4 + 2i,  4 + 3i,  4 + 0i];

% Calculate all the eigenvalues and eigenvectors of A
job = 'Vectors';
[z, w, info] = f08fq( ...
                     job, uplo, a);

% Normalize vectors, largest element is real and positive.
for i = 1:n
  [~,k] = max(abs(real(z(:,i)))+abs(imag(z(:,i))));
  z(:,i) = z(:,i)*conj(z(k,i))/abs(z(k,i));
end

% Display results
fprintf('Eigenvalues:\n');
disp(w);

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

9.2 Program Results

```
     f08fq example results

Eigenvalues:
   -4.2443
   -0.6886
    1.1412
   13.7916

 Eigenvectors
                     1                  2                  3                  4
 1  (-0.3839,-0.2941) ( 0.6470, 0.0000) (-0.4326, 0.1068) ( 0.3309,-0.1986)
 2  (-0.4512, 0.1102) (-0.4984,-0.1130) (-0.1590,-0.5480) ( 0.3728,-0.2419)
 3  ( 0.0263, 0.4857) ( 0.2949, 0.3165) ( 0.5491, 0.0000) ( 0.4870,-0.1938)
 4  ( 0.5602, 0.0000) (-0.2241,-0.2878) (-0.2865, 0.3037) ( 0.6155, 0.0000)
```