NAG Toolbox

nag_lapack_dsbev (f08ha)

1 Purpose

nag_lapack_dsbev (f08ha) computes all the eigenvalues and, optionally, all the eigenvectors of a real n by n symmetric band matrix A of bandwidth $(2k_d + 1)$.

2 Syntax

```
[ab, w, z, info] = nag_lapack_dsbev(jobz, uplo, kd, ab, 'n', n)
[ab, w, z, info] = f08ha(jobz, uplo, kd, ab, 'n', n)
```

3 Description

The symmetric band matrix A is first reduced to tridiagonal form, using orthogonal 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 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: **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: **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'.

3: **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.

4: **ab**$(ldab,:)$ – REAL (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 symmetric 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 $j \leq i \leq \min(n, j + k_d)$.

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

The first dimension of the array **ab** will be **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: **w**$(\mathbf{n})$ – REAL (KIND=nag_wp) array

The eigenvalues in ascending order.

3: **z**$(ldz,:)$ – REAL (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 $\max(1,\mathbf{n})$ if **jobz** $=$ 'V' and 1 otherwise.

If **jobz** $=$ 'V', **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.

4: **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: **uplo**, 3: **n**, 4: **kd**, 5: **ab**, 6: **ldab**, 7: **w**, 8: **z**, 9: **ldz**, 10: **work**, 11: **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** $= i$, 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

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

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 complex analogue of this function is nag_lapack_zhbev (f08hn).

9 Example

This example finds all the eigenvalues and eigenvectors of the symmetric band matrix

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

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

9.1 Program Text

```
function f08ha_example

fprintf('f08ha example results\n\n');

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

% Calculate all eigenvalues and eigenvectors
jobz = 'Vectors';
[abf, w, z, info] = f08ha( ...
                           jobz, uplo, kd, ab);

% Normalize eigenvectors: largest element positive
for j = 1:n
  [~,k] = max(abs(z(:,j)));
  if z(k,j) < 0;
    z(:,j) = -z(:,j);
  end
end

disp('Eigenvalues');
disp(w);
```

```
disp('Eigenvectors');
disp(z);

% Eigenvalue error bound
errbnd = x02aj*max(abs(w(1)),abs(w(end)));
% Eigenvector condition numbers
[rcondz, info] = f08fl( ...
         'Eigenvectors', n, n, w);

% Eigenvector error bounds
zerrbd = errbnd./rcondz;

disp('Error estimate for the eigenvalues');
fprintf('%12.1e\n',errbnd);
disp('Error estimates for the eigenvectors');
fprintf('%12.1e',zerrbd);
fprintf('\n');
```

9.2 Program Results

```
     f08ha example results

Eigenvalues
   -3.2474
   -2.6633
    1.7511
    4.1599
   14.9997

Eigenvectors
    0.0394    0.6238    0.5635   -0.5165    0.1582
    0.5721   -0.2575   -0.3896   -0.5955    0.3161
   -0.4372   -0.5900    0.4008   -0.1470    0.5277
   -0.4424    0.4308   -0.5581    0.0470    0.5523
    0.5332    0.1039    0.2421    0.5956    0.5400

Error estimate for the eigenvalues
     1.7e-15
Error estimates for the eigenvectors
     2.9e-15     2.9e-15     6.9e-16     6.9e-16     1.5e-16
```