NAG Toolbox

nag_lapack_dspevx (f08gb)

1 Purpose

nag_lapack_dspevx (f08gb) computes selected eigenvalues and, optionally, eigenvectors of a real n by n symmetric matrix A in packed storage. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Syntax

```
[ap, m, w, z, jfail, info] = nag_lapack_dspevx(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol)
[ap, m, w, z, jfail, info] = f08gb(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol)
```

3 Description

The symmetric matrix A is first reduced to tridiagonal form, using orthogonal 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: **n** – INTEGER

n, the order of the matrix A.

Constraint: **n** ≥ 0.

5: **ap**(:) – REAL (KIND=nag_wp) array

The dimension of the array **ap** must be at least $\max(1, \mathbf{n} \times (\mathbf{n}+1)/2)$

The upper or lower triangle of the n by n symmetric matrix A, packed by columns.

More precisely,

if **uplo** = 'U', the upper triangle of A must be stored with element A_{ij} in **ap**$(i + j(j-1)/2)$ for $i \leq j$;

if **uplo** = 'L', the lower triangle of A must be stored with element A_{ij} in **ap**$(i + (2n-j)(j-1)/2)$ for $i \geq j$.

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

None.

5.3 Output Parameters

1: **ap**(:) – REAL (KIND=nag_wp) array

The dimension of the array **ap** will be $\max(1, \mathbf{n} \times (\mathbf{n}+1)/2)$

ap stores the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.

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**(**n**) – REAL (KIND=nag_wp) array

The selected eigenvalues in ascending order.

4: **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 $\max(1, \mathbf{m})$ 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.

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 complex analogue of this function is nag_lapack_zhpevx (f08gp).

9 Example

This example finds the eigenvalues in the half-open interval $(-1, 1]$, and the corresponding eigenvectors, of the symmetric matrix

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

9.1 Program Text

```
function f08gb_example

fprintf('f08gb example results\n\n');

% Eigenvalues in range [-1,1] of symmetric A stored in packed format.
n  = nag_int(4);
ap = [1;
      2;     2;
      3;     3;     3;
      4;     4;     4;     4];

jobz  = 'Vectors';
range = 'Values in range';
uplo  = 'U';
vl = -1;
vu =  1;
il = nag_int(0);
iu = nag_int(0);
abstol = 0;
[~, m, w, z, jfail, info] = ...
f08gb( ...
       jobz, range, uplo, n, ap, vl, vu, il, iu, abstol);

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

disp(' Eigenvalues of A in range:');
disp(w(1:m));
disp(' Corresponding eigenvectors:');
disp(z);
```

9.2 Program Results

```
     f08gb example results

 Eigenvalues of A in range:
   -0.5146
   -0.2943

 Corresponding eigenvectors:
   -0.5144   -0.2767
    0.4851    0.6634
    0.5420   -0.6504
   -0.4543    0.2457
```