NAG Toolbox for MATLAB

f08gp

1 Purpose

f08gp computes selected eigenvalues and, optionally, eigenvectors of a complex n by n Hermitian 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] = f08gp(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol)
```

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 URL: 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 – string
```

If jobz = 'N', compute eigenvalues only.

If jobz = 'V', compute eigenvalues and eigenvectors.

Constraint: jobz = 'N' or 'V'.

2: range – string

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

If range = 'V', all eigenvalues in the half-open interval (vl, vu] will be found.

If range = 'I', the ilth to iuth eigenvalues will be found.

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

3: **uplo – string**

If $\mathbf{uplo} = 'U'$, the upper triangular part of A is stored.

If uplo = 'L', the lower triangular part of A is stored.

Constraint: uplo = 'U' or 'L'.

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4: n - int32 scalar

n, the order of the matrix A.

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

5: ap(*) – complex array

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

The n by n Hermitian matrix A, packed by columns.

More precisely,

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

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

6: vl – double scalar

7: **vu – double scalar**

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 – int32 scalar

9: iu – int32 scalar

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
$$\mathbf{n} = 0$$
, $\mathbf{il} = 1$ and $\mathbf{iu} = 0$;
if $\mathbf{n} > 0$, $1 \le \mathbf{il} \le \mathbf{iu} \le \mathbf{n}$.

10: abstol – double scalar

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

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 \text{x02am}(\)$, not zero. If this function returns with **info** > 0, indicating that some eigenvectors did not converge, try setting **abstol** to $2 \times \text{x02am}(\)$. See Demmel and Kahan 1990.

5.2 Optional Input Parameters

None.

5.3 Input Parameters Omitted from the MATLAB Interface

ldz, work, rwork, iwork

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5.4 Output Parameters

1: ap(*) – complex array

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

ap contains 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 - int32 scalar

The total number of eigenvalues found.

If range =
$$'A'$$
, $m = n$.

If range = 'V', the exact value of m is not known in advance, but will satisfy $0 \le m \le n$.

If range = 'I',
$$\mathbf{m} = \mathbf{i}\mathbf{u} - \mathbf{i}\mathbf{l} + 1$$
.

3: $\mathbf{w}(*)$ – double array

Note: the dimension of the array w must be at least $max(1, \mathbf{n})$.

If info = 0, the selected eigenvalues in ascending order.

4: z(ldz,*) – complex array

The first dimension, ldz, of the array z must satisfy

if
$$jobz = 'V'$$
, $ldz \ge max(1, n)$; $ldz \ge 1$ otherwise.

The second dimension of the array must be at least $max(1, \mathbf{m})$ if $\mathbf{jobz} = 'V'$, and at least 1 otherwise

If $\mathbf{jobz} = 'V'$, then if $\mathbf{info} = 0$, 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, then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in **jfail**.

```
If jobz = 'E', z is not referenced.
```

Note: you must ensure that at least $max(1, \mathbf{m})$ columns are supplied in the array \mathbf{z} ; if $\mathbf{range} = 'V'$, the exact value of \mathbf{m} is not known in advance and an upper bound must be used.

5: jfail(*) - int32 array

Note: the dimension of the array **ifail** must be at least $max(1, \mathbf{n})$.

If jobz = 'V', then if info = 0, the first m elements of jfail are zero.

If info > 0, ifail contains the indices of the eigenvectors that failed to converge.

If jobz = 'E', **jfail** is not referenced.

6: info – int32 scalar

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

6 Error Indicators and Warnings

Errors or warnings detected by the function:

$$info = -i$$

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

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1: jobz, 2: range, 3: uplo, 4: n, 5: ap, 6: vl, 7: vu, 8: il, 9: iu, 10: abstol, 11: m, 12: w, 13: z, 14: ldz, 15: work, 16: rwork, 17: iwork, 18: jfail, 19: 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, then i eigenvectors failed to converge. Their indices are stored in array info please see info 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 n^3 .

The real analogue of this function is f08gb.

9 Example

```
jobz = 'Vectors';
range = 'Values in range';
uplo = 'U';
n = int32(4);
ap = [complex(1, +0);
     complex(2, -1);
complex(2, +0);
     complex(3, -1);
     complex(3, -2);
     complex(3, +0);
     complex(4, -1);
     complex(4, -2);
complex(4, -3);
     complex(4, +0)];
v1 = -2;
vu = 2;
il = int32(-1208245600);
iu = int32(121387641);
abstol = 0;
[apOut, m, w, z, jfail, info] = f08gp(jobz, range, uplo, n, ap, v1, vu,
il, iu, abstol)
apOut =
  -0.2187
   1.0422
  -0.3942
   0.4448 + 0.4277i
  -3.4564
   6.6129
   0.3367 + 0.0008i
   0.3567 - 0.0783i
  -7.8740
   4.0000
m =
            2
w =
```

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