# **NAG Toolbox for MATLAB**

# f08qg

# 1 Purpose

f08qg reorders the Schur factorization of a real general matrix so that a selected cluster of eigenvalues appears in the leading elements or blocks on the diagonal of the Schur form. The function also optionally computes the reciprocal condition numbers of the cluster of eigenvalues and/or the invariant subspace.

## 2 Syntax

[t, q, wr, wi, m, s, sep, info] = 
$$f08qg(job, compq, select, t, q, 'n', n)$$

## 3 Description

f08qg reorders the Schur factorization of a real general matrix  $A = QTQ^{T}$ , so that a selected cluster of eigenvalues appears in the leading diagonal elements or blocks of the Schur form.

The reordered Schur form  $\tilde{T}$  is computed by an orthogonal similarity transformation:  $\tilde{T} = Z^T T Z$ . Optionally the updated matrix  $\tilde{Q}$  of Schur vectors is computed as  $\tilde{Q} = Q Z$ , giving  $A = \tilde{Q} \tilde{T} \tilde{Q}^T$ .

Let  $\tilde{T} = \begin{pmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{pmatrix}$ , where the selected eigenvalues are precisely the eigenvalues of the leading m by m

sub-matrix  $T_{11}$ . Let  $\tilde{Q}$  be correspondingly partitioned as  $(Q_1 \ Q_2)$  where  $Q_1$  consists of the first m columns of Q. Then  $AQ_1 = Q_1T_{11}$ , and so the m columns of  $Q_1$  form an orthonormal basis for the invariant subspace corresponding to the selected cluster of eigenvalues.

Optionally the function also computes estimates of the reciprocal condition numbers of the average of the cluster of eigenvalues and of the invariant subspace.

### 4 References

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 – string

Indicates whether condition numbers are required for the cluster of eigenvalues and/or the invariant subspace.

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```
job = 'N'
```

No condition numbers are required.

job = 'E'

Only the condition number for the cluster of eigenvalues is computed.

job = 'V'

Only the condition number for the invariant subspace is computed.

job = 'B'

Condition numbers for both the cluster of eigenvalues and the invariant subspace are computed.

Constraint: job = 'N', 'E', 'V' or 'B'.

### 2: **compq – string**

Indicates whether the matrix Q of Schur vectors is to be updated.

$$compq = 'V'$$

The matrix Q of Schur vectors is updated.

compq = 'N'

No Schur vectors are updated.

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

## 3: select(\*) - logical array

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

The eigenvalues in the selected cluster. To select a real eigenvalue  $\lambda_j$ , select(j) must be set true. To select a complex conjugate pair of eigenvalues  $\lambda_j$  and  $\lambda_{j+1}$  (corresponding to a 2 by 2 diagonal block), select(j) and/or select(j+1) must be set to true. A complex conjugate pair of eigenvalues must be either both included in the cluster or both excluded. See also Section 8.

### 4: t(ldt,\*) – double array

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

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

The n by n upper quasi-triangular matrix T in canonical Schur form, as returned by f08pe. See also Section 8.

### 5: q(ldq,\*) - double array

The first dimension, **ldq**, of the array **q** must satisfy

```
if compq = 'V', ldq \ge max(1, n); if compq = 'N', ldq \ge 1.
```

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

If compq = 'V', q must contain the n by n orthogonal matrix Q of Schur vectors, as returned by f08pe.

### 5.2 Optional Input Parameters

#### 1: n - int32 scalar

Default: The dimension of the array select The second dimension of the array t.

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n, the order of the matrix T.

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

## 5.3 Input Parameters Omitted from the MATLAB Interface

ldt, ldq, work, lwork, iwork, liwork

### 5.4 Output Parameters

### 1: t(ldt,\*) - double array

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

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

**t** contains the updated matrix  $\tilde{T}$ .

### 2: q(ldq,\*) - double array

The first dimension, Idq, of the array q must satisfy

```
if compq = 'V', ldq \ge max(1, n); if compq = 'N', ldq \ge 1.
```

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

If compq = 'V', q contains the updated matrix of Schur vectors; the first m columns of Q form an orthonormal basis for the specified invariant subspace.

If compq = 'N', q is not referenced.

#### 3: wr(\*) – double array

### 4: wi(\*) – double array

**Note**: the dimension of the arrays wr and wi must be at least  $max(1, \mathbf{n})$ .

The real and imaginary parts, respectively, of the reordered eigenvalues of  $\tilde{T}$ . The eigenvalues are stored in the same order as on the diagonal of  $\tilde{T}$ ; see Section 8 for details. Note that if a complex eigenvalue is sufficiently ill-conditioned, then its value may differ significantly from its value before reordering.

### 5: m - int32 scalar

m, the dimension of the specified invariant subspace. The value of m is obtained by counting 1 for each selected real eigenvalue and 2 for each selected complex conjugate pair of eigenvalues (see **select**);  $0 \le m \le n$ .

#### 6: s - double scalar

If  $\mathbf{job} = 'E'$  or 'B',  $\mathbf{s}$  is a lower bound on the reciprocal condition number of the average of the selected cluster of eigenvalues. If  $\mathbf{m} = 0$  or  $\mathbf{n}$ ,  $\mathbf{s} = 1$ ; if  $\mathbf{info} = 1$  (see Section 6),  $\mathbf{s}$  is set to zero.

If job = 'N' or 'V', s is not referenced.

#### 7: sep – double scalar

If  $\mathbf{job} = 'V'$  or 'B',  $\mathbf{sep}$  is the estimated reciprocal condition number of the specified invariant subspace. If  $\mathbf{m} = 0$  or  $\mathbf{n}$ ,  $\mathbf{sep} = ||T||$ ; if  $\mathbf{info} = 1$  (see Section 6),  $\mathbf{sep}$  is set to zero.

If job = 'N' or 'E', sep is not referenced.

### 8: info – int32 scalar

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

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## 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:

1: job, 2: compq, 3: select, 4: n, 5: t, 6: ldt, 7: q, 8: ldq, 9: wr, 10: wi, 11: m, 12: s, 13: sep, 14: work, 15: lwork, 16: iwork, 17: liwork, 18: 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 = 1

The reordering of T failed because a selected eigenvalue was too close to an eigenvalue which was not selected; this error exit can only occur if at least one of the eigenvalues involved was complex. The problem is too ill-conditioned: consider modifying the selection of eigenvalues so that eigenvalues which are very close together are either all included in the cluster or all excluded. On exit, T may have been partially reordered, but  $\mathbf{wr}$ ,  $\mathbf{wi}$  and Q (if requested) are updated consistently with T;  $\mathbf{s}$  and  $\mathbf{sep}$  (if requested) are both set to zero.

## 7 Accuracy

The computed matrix  $\tilde{T}$  is similar to a matrix (T+E), where

$$||E||_2 = O(\epsilon)||T||_2$$

and  $\epsilon$  is the *machine precision*.

s cannot underestimate the true reciprocal condition number by more than a factor of  $\sqrt{\min(m,n-m)}$ . sep may differ from the true value by  $\sqrt{m(n-m)}$ . The angle between the computed invariant subspace and the true subspace is  $\frac{O(\epsilon)\|A\|_2}{sep}$ .

Note that if a 2 by 2 diagonal block is involved in the reordering, its off-diagonal elements are in general changed; the diagonal elements and the eigenvalues of the block are unchanged unless the block is sufficiently ill-conditioned, in which case they may be noticeably altered. It is possible for a 2 by 2 block to break into two 1 by 1 blocks, that is, for a pair of complex eigenvalues to become purely real. The values of real eigenvalues however are never changed by the reordering.

### **8** Further Comments

The input matrix T must be in canonical Schur form, as is the output matrix  $\tilde{T}$ . This has the following structure.

If all the computed eigenvalues are real,  $\tilde{T}$  is upper triangular, and the diagonal elements of  $\tilde{T}$  are the eigenvalues;  $\mathbf{wr}(i) = \tilde{t}_{ii}$  for i = 1, 2, ..., n and  $\mathbf{wi}(i) = 0.0$ .

If some of the computed eigenvalues form complex conjugate pairs, then  $\tilde{T}$  has 2 by 2 diagonal blocks. Each diagonal block has the form

$$\begin{pmatrix} \tilde{t}_{ii} & \tilde{t}_{i,i+1} \\ \tilde{t}_{i+1,i} & \tilde{t}_{i+1,i+1} \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \alpha \end{pmatrix}$$

where  $\beta \gamma < 0$ . The corresponding eigenvalues are  $\alpha \pm \sqrt{\beta \gamma}$ ;  $\mathbf{wr}(i) = \mathbf{wr}(i+1) = \alpha$ ;  $\mathbf{wi}(i) = +\sqrt{|\beta \gamma|}$ ;  $\mathbf{wi}(i+1) = -\mathbf{wi}(i)$ .

The complex analogue of this function is f08qu.

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# 9 Example

```
job = 'Both';
compq = 'Vectors';
select = [true;
     false;
     false;
     true];
t = [0.7995, -0.1144, 0.006, 0.0336;
     0, -0.0994, 0.2478, 0.3474;
     0, -0.6483, -0.0994, 0.2026;
0, 0, 0, -0.1007];
q = [0.6551, 0.1037, 0.345, 0.6641;
     0.5236, -0.5807, -0.6141, -0.1068; -0.5362, -0.3073, -0.2935, 0.729299999999999;
0.0956, 0.7467, -0.6463, 0.1249]; [tOut, qOut, wr, wi, m, s, sep, info] = f08qg(job, compq, select, t, q)
tOut =
    0.7995
              0.0059
                        -0.0751
                                    0.0927
          0
              -0.1007
                         -0.3936
                                     0.3569
          0
                     0
                         -0.0994
                                     0.5128
                                   -0.0994
          0
                     0
                        -0.3133
qOut =
              -0.1211
    0.6551
                          0.5032
                                     0.5504
    0.5236
              -0.3286
                          -0.7857
                                      0.0228
              -0.5974
   -0.5362
                         -0.0904
                                      0.5894
    0.0956
              -0.7215
                         0.3482
                                     -0.5908
wr =
    0.7995
   -0.1007
   -0.0994
   -0.0994
wi =
          0
          0
    0.4008
   -0.4008
m =
   0.5699
sep =
    0.3102
info =
            0
```

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