NAG Toolbox for MATLAB

f08pe

1 Purpose

f08pe computes all the eigenvalues and, optionally, the Schur factorization of a real Hessenberg matrix or a real general matrix which has been reduced to Hessenberg form.

2 Syntax

[h, wr, wi, z, info] =
$$f08pe(job, compz, ilo, ihi, h, z, 'n', n)$$

3 Description

f08pe computes all the eigenvalues and, optionally, the Schur factorization of a real upper Hessenberg matrix H:

$$H = ZTZ^{\mathrm{T}}$$
,

where T is an upper quasi-triangular matrix (the Schur form of H), and Z is the orthogonal matrix whose columns are the Schur vectors z_i . See Section 8 for details of the structure of T.

The function may also be used to compute the Schur factorization of a real general matrix A which has been reduced to upper Hessenberg form H:

$$A = QHQ^{T}$$
, where Q is orthogonal,
= $(QZ)T(QZ)^{T}$.

In this case, after f08ne has been called to reduce A to Hessenberg form, f08nf must be called to form Q explicitly; Q is then passed to f08pe, which must be called with **compz** = 'V'.

The function can also take advantage of a previous call to f08nh which may have balanced the original matrix before reducing it to Hessenberg form, so that the Hessenberg matrix H has the structure:

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} \\ & H_{22} & H_{23} \\ & & H_{33} \end{pmatrix}$$

where H_{11} and H_{33} are upper triangular. If so, only the central diagonal block H_{22} (in rows and columns i_{lo} to i_{hi}) needs to be further reduced to Schur form (the blocks H_{12} and H_{23} are also affected). Therefore the values of i_{lo} and i_{hi} can be supplied to f08pe directly. Also, f08nj must be called after this function to permute the Schur vectors of the balanced matrix to those of the original matrix. If f08nh has not been called however, then i_{lo} must be set to 1 and i_{hi} to n. Note that if the Schur factorization of A is required, f08nh must **not** be called with **job** = 'S' or 'B', because the balancing transformation is not orthogonal.

f08pe uses a multishift form of the upper Hessenberg QR algorithm, due to Bai and Demmel 1989. The Schur vectors are normalized so that $||z_i||_2 = 1$, but are determined only to within a factor ± 1 .

4 References

Bai Z and Demmel J W 1989 On a block implementation of Hessenberg multishift *QR* iteration *Internat. J. High Speed Comput.* **1** 97–112

Golub G H and Van Loan C F 1996 Matrix Computations (3rd Edition) Johns Hopkins University Press, Baltimore

[NP3663/21] f08pe.1

f08pe NAG Toolbox Manual

5 Parameters

5.1 Compulsory Input Parameters

1: **job** – **string**

Indicates whether eigenvalues only or the Schur form T is required.

$$job = 'E'$$

Eigenvalues only are required.

$$job = 'S'$$

The Schur form T is required.

Constraint: job = 'E' or 'S'.

2: compz – string

Indicates whether the Schur vectors are to be computed.

$$compz = 'N'$$

No Schur vectors are computed (and the array z is not referenced).

$$compz = 'I'$$

The Schur vectors of H are computed (and the array z is initialized by the function).

$$compz = 'V'$$

The Schur vectors of A are computed (and the array \mathbf{z} must contain the matrix Q on entry).

Constraint: compz = 'N', 'V' or 'I'.

- 3: ilo int32 scalar
- 4: ihi int32 scalar

If the matrix A has been balanced by f08nh, then **ilo** and **ihi** must contain the values returned by that function. Otherwise, **ilo** must be set to 1 and **ihi** to **n**.

Constraint: ilo ≥ 1 and min(ilo, n) \leq ihi \leq n.

5: h(ldh,*) - double array

The first dimension of the array **h** 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 Hessenberg matrix H, as returned by f08ne.

6: z(ldz,*) – double array

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

```
if compz = 'V' or 'I', ldz \ge max(1, n); if compz = 'N', ldz \ge 1.
```

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

If compz = 'V', z must contain the orthogonal matrix Q from the reduction to Hessenberg form.

If compz = 'I', z need not be set.

f08pe.2 [NP3663/21]

5.2 Optional Input Parameters

1: n - int32 scalar

Default: The first dimension of the array \mathbf{h} and the second dimension of the array \mathbf{h} . (An error is raised if these dimensions are not equal.)

n, the order of the matrix H.

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

5.3 Input Parameters Omitted from the MATLAB Interface

ldh, ldz, work, lwork

5.4 Output Parameters

1: h(ldh,*) - double array

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

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

If job = 'E', the array contains no useful information.

If $\mathbf{job} = 'S'$, **h** contains the upper quasi-triangular matrix T from the Schur decomposition (the Schur form) unless $\mathbf{info} > 0$.

- 2: wr(*) double array
- 3: wi(*) double array

Note: the dimension of the arrays wr and wi must be at least max(1, n).

The real and imaginary parts, respectively, of the computed eigenvalues, unless **info** > 0 (in which case see Section 6). Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first. The eigenvalues are stored in the same order as on the diagonal of the Schur form T (if computed); see Section 8 for details.

4: $z(ldz_{\bullet}*)$ – double array

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

```
if compz = 'V' or 'I', ldz \ge max(1, n); if compz = 'N', ldz \ge 1.
```

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

If compz = 'V' or 'I', z contains the orthogonal matrix of the required Schur vectors, unless info > 0.

If compz = 'N', z is not referenced.

5: 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 $\mathbf{info} = -i$, parameter i had an illegal value on entry. The parameters are numbered as follows: 1: \mathbf{job} , 2: \mathbf{compz} , 3: \mathbf{n} , 4: \mathbf{ilo} , 5: \mathbf{ihi} , 6: \mathbf{h} , 7: \mathbf{ldh} , 8: \mathbf{wr} , 9: \mathbf{wi} , 10: \mathbf{z} , 11: \mathbf{ldz} , 12: \mathbf{work} , 13: \mathbf{lwork} , 14: \mathbf{info} .

[NP3663/21] f08pe.3

f08pe NAG Toolbox Manual

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

The algorithm has failed to find all the eigenvalues after a total of $30 \times (\mathbf{ihi} - \mathbf{ilo} + 1)$ iterations. If $\mathbf{info} = i$, elements $1, 2, \dots, \mathbf{ilo} - 1$ and $i + 1, i + 2, \dots, n$ of \mathbf{wr} and \mathbf{wi} contain the real and imaginary parts of contain the eigenvalues which have been found.

If job = 'E', then on exit, the remaining unconverged eigenvalues are the eigenvalues of the upper Hessenberg matrix rows and columns of **ilo** through **info** of the final, output value of H.

If job = 'S', then on exit

(*) (initial value of
$$H$$
) * $U = U$ * (final value of H)

where U is an orthogonal matrix. The final value of H is upper Hessenberg and quasi-triangular in rows and columns info + 1 through ihi.

If compz = 'V', then on exit

(final value of
$$Z$$
) = (initial value of Z) * U

where U is the orthogonal matrix in (*) (regardless of the value of **job**).

If compz = 'I', then on exit

(final value of
$$Z$$
) = U

where U is the orthogonal matrix in (*) (regardless of the value of **job**).

If info > 0 and compz = 'N', then z is not accessed.

7 Accuracy

The computed Schur factorization is the exact factorization of a nearby matrix (H + E), where

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

and ϵ is the *machine precision*.

If λ_i is an exact eigenvalue, and $\tilde{\lambda}_i$ is the corresponding computed value, then

$$\left|\tilde{\lambda}_i - \lambda_i\right| \le \frac{c(n)\epsilon \|H\|_2}{s_i},$$

where c(n) is a modestly increasing function of n, and s_i is the reciprocal condition number of λ_i . The condition numbers s_i may be computed by calling f08ql.

8 Further Comments

The total number of floating-point operations depends on how rapidly the algorithm converges, but is typically about:

 $7n^3$ if only eigenvalues are computed;

 $10n^3$ if the Schur form is computed;

 $20n^3$ if the full Schur factorization is computed.

The Schur form T has the following structure (referred to as **canonical** Schur form).

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

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

f08pe.4 [NP3663/21]

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

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 f08ps.

9 Example

```
job = 'Schur form';
compz = 'Initialize Z';
ilo = int32(1);
ihi = int32(4);
h = [0.35, -0.116, -0.3886, -0.2942;
     -0.514, 0.1225, 0.1004, 0.1126;
    0, 0.6443, -0.1357, -0.0977;
0, 0, 0.4262, 0.1632];
z = zeros(4, 4);
[hOut, wr, wi, zOut, info] = f08pe(job, compz, ilo, ihi, h, z)
hOut =
    0.7995
             0.0061
                      -0.1144
                                -0.0335
            -0.0994 -0.6483
                               -0.2026
        0
            0.2477 -0.0994 -0.3474
                0
                          0 -0.1007
wr =
   0.7995
   -0.0994
   -0.0994
   -0.1007
   0.4008
  -0.4008
zOut =
  -0.6551
            -0.3450 -0.1036 0.6641
   0.5972
            -0.1706 0.5246 0.5823
                               -0.0821
   0.3845
            -0.7143 -0.5789
    0.2576
            0.5845
                     -0.6156
                                 0.4616
info =
          0
```

[NP3663/21] f08pe.5 (last)