F08PKF (SHSEIN/DHSEIN) – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

F08PKF (SHSEIN/DHSEIN) computes selected left and/or right eigenvectors of a real upper Hessenberg matrix corresponding to specified eigenvalues, by inverse iteration.

2 Specification

```
 SUBROUTINE F08PKF(JOB, EIGSRC, INITV, SELECT, N, H, LDH, WR, WI,
1                  VL, LDVL, VR, LDVR, MM, M, WORK, IFAILL, IFAILR,
2                  INFO)
 ENTRY      shsein(JOB, EIGSRC, INITV, SELECT, N, H, LDH, WR, WI,
1                  VL, LDVL, VR, LDVR, MM, M, WORK, IFAILL, IFAILR,
2                  INFO)
 INTEGER           N, LDH, LDVL, LDVR, MM, M, IFAILL(*), IFAILR(*),
1                  INFO
 real              H(LDH,*), WR(*), WI(*), VL(LDVL,*), VR(LDVR,*),
1                  WORK(*)
 LOGICAL           SELECT(*)
 CHARACTER*1       JOB, EIGSRC, INITV
```

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine computes left and/or right eigenvectors of a real upper Hessenberg matrix H, corresponding to selected eigenvalues.

The right eigenvector x, and the left eigenvector y, corresponding to an eigenvalue λ, are defined by:

$$Hx = \lambda x \text{ and } y^H H = \lambda y^H \text{ (or } H^T y = \bar{\lambda} y).$$

Note that even though H is real, λ, x and y may be complex. If x is an eigenvector corresponding to a complex eigenvalue λ, then the complex conjugate vector $\bar{x}$ is the eigenvector corresponding to the complex conjugate eigenvalue $\bar{\lambda}$.

The eigenvectors are computed by inverse iteration. They are scaled so that, for a real eigenvector x, $\max(|x_i|) = 1$, and for a complex eigenvector, $\max(|\mathrm{Re}(x_i)| + |\mathrm{Im}(x_i)|) = 1$.

If H has been formed by reduction of a real general matrix A to upper Hessenberg form, then eigenvectors of H may be transformed to eigenvectors of A by a call to F08NGF (SORMHR/DORMHR).

4 References

[1] Golub G H and van Loan C F (1996) *Matrix Computations* Johns Hopkins University Press (3rd Edition), Baltimore

5 Parameters

1: JOB — CHARACTER*1 *Input*

On entry: indicates whether left and/or right eigenvectors are to be computed as follows:

if JOB = 'R', then only right eigenvectors are computed;
if JOB = 'L', then only left eigenvectors are computed;

if JOB = 'B', then both left and right eigenvectors are computed.

Constraint: JOB = 'R', 'L' or 'B'.

2: EIGSRC — CHARACTER*1 *Input*

On entry: indicates whether the eigenvalues of H (stored in WR and WI) were found using F08PEF (SHSEQR/DHSEQR) as follows:

if EIGSRC = 'Q', then the eigenvalues of H were found using F08PEF (SHSEQR/DHSEQR); thus if H has any zero sub-diagonal elements (and so is block triangular), then the jth eigenvalue can be assumed to be an eigenvalue of the block containing the jth row/column. This property allows the routine to perform inverse iteration on just one diagonal block;

if EIGSRC = 'N', then no such assumption is made and the routine performs inverse iteration using the whole matrix.

Constraint: EIGSRC = 'Q' or 'N'.

3: INITV — CHARACTER*1 *Input*

On entry: indicates whether the user is supplying initial estimates for the selected eigenvectors as follows:

if INITV = 'N', then no initial estimates are supplied;

if INITV = 'U', then initial estimates are supplied in VL and/or VR.

Constraint: INITV = 'N' or 'U'.

4: SELECT($*$) — LOGICAL array *Input/Output*

Note: the dimension of the array SELECT must be at least max(1,N).

On entry: SELECT specifies which eigenvectors are to be computed. To obtain the real eigenvector corresponding to the real eigenvalue WR(j), SELECT(j) must be set .TRUE.. To select the complex eigenvector corresponding to the complex eigenvalue (WR(j),WI}(j)) with complex conjugate (WR($j+1$),WI($j+1$)), SELECT(j) and/or SELECT($j+1$) must be set .TRUE.; the eigenvector corresponding to the **first** eigenvalue in the pair is computed.

On exit: if a complex eigenvector was selected as specified above, then SELECT(j) is set to .TRUE. and SELECT($j+1$) to .FALSE..

5: N — INTEGER *Input*

On entry: n, the order of the matrix H.

Constraint: N $\geq$ 0.

6: H(LDH,$*$) — ***real*** array *Input*

Note: the second dimension of the array H must be at least max(1,N).

On entry: the n by n upper Hessenberg matrix H.

7: LDH — INTEGER *Input*

On entry: the first dimension of the array H as declared in the (sub)program from which F08PKF (SHSEIN/DHSEIN) is called.

Constraint: LDH $\geq$ max(1,N).

8: WR($*$) — ***real*** array *Input/Output*

Note: the dimension of the array WR must be at least max(1,N).

9: WI(∗) — ***real*** array *Input*

Note: the dimension of the array WI must be at least max(1,N).

On entry: the real and imaginary parts, respectively, of the eigenvalues of the matrix H. Complex conjugate pairs of values must be stored in consecutive elements of the arrays. If EIGSRC = 'Q', the arrays **must** be exactly as returned by F08PEF (SHSEQR/DHSEQR).

On exit: some elements of WR may be modified, as close eigenvalues are perturbed slightly in searching for independent eigenvectors.

10: VL(LDVL,∗) — ***real*** array *Input/Output*

Note: the second dimension of the array VL must be at least max(1,MM) if JOB = 'L' or 'B' and at least 1 if JOB = 'R' .

On entry: if INITV = 'U' and JOB = 'L' or 'B', VL must contain starting vectors for inverse iteration for the left eigenvectors. Each starting vector must be stored in the same column or columns as will be used to store the corresponding eigenvector (see below). If INITV = 'N', VL need not be set.

On exit: if JOB = 'L' or 'B', VL contains the computed left eigenvectors (as specified by SELECT). The eigenvectors are stored consecutively in the columns of the array, in the same order as their eigenvalues. Corresponding to each selected real eigenvalue is a real eigenvector, occupying one column. Corresponding to each selected complex eigenvalue is a complex eigenvector, occupying two columns: the first column holds the real part and the second column holds the imaginary part.

VL is not referenced if JOB = 'R'.

11: LDVL — INTEGER *Input*

On entry: the first dimension of the array VL as declared in the (sub)program from which F08PKF (SHSEIN/DHSEIN) is called.

Constraints:

LDVL $\geq$ max(1,N) if JOB = 'L' or 'B',
LDVL $\geq$ 1 if JOB = 'R'.

12: VR(LDVR,∗) — ***real*** array *Input/Output*

Note: the second dimension of the array VR must be at least max(1,MM) if JOB = 'R' or 'B' and at least 1 if JOB = 'L'.

On entry: if INITV = 'U' and JOB = 'R' or 'B', VR must contain starting vectors for inverse iteration for the right eigenvectors. Each starting vector must be stored in the same column or columns as will be used to store the corresponding eigenvector (see below). If INITV = 'N', VR need not be set.

On exit: if JOB = 'R' or 'B', VR contains the computed right eigenvectors (as specified by SELECT). The eigenvectors are stored consecutively in the columns of the array, in the same order as their eigenvalues. Corresponding to each selected real eigenvalue is a real eigenvector, occupying one column. Corresponding to each selected complex eigenvalue is a complex eigenvector, occupying two columns: the first column holds the real part and the second column holds the imaginary part.

VR is not referenced if JOB = 'L'.

13: LDVR — INTEGER *Input*

On entry: the first dimension of the array VR as declared in the (sub)program from which F08PKF (SHSEIN/DHSEIN) is called.

Constraints:

LDVR $\geq$ max(1,N) if JOB = 'R' or 'B',
LDVR $\geq$ 1 if JOB = 'L'.

14: MM — INTEGER *Input*

On entry: the number of columns in the arrays VL and/or VR. The actual number of columns required, m, is obtained by counting 1 for each selected real eigenvector and 2 for each selected complex eigenvector (see SELECT); $0 \le m \le n$.

Constraint: MM $\ge m$.

15: M — INTEGER *Output*

On exit: m, the number of columns of VL and/or VR required to store the selected eigenvectors.

16: WORK(*) — ***real*** array *Workspace*

Note: the dimension of the array WORK must be at least max(1,N*(N+2)).

17: IFAILL(*) — INTEGER array *Output*

Note: the dimension of the array IFAILL must be at least max(1,MM) if JOB = 'L' or 'B' and at least 1 if JOB = 'R'.

On exit: if JOB = 'L' or 'B', then IFAILL(i) = 0 if the selected left eigenvector converged and IFAILL(i) = $j > 0$ if the eigenvector stored in the ith column of VL (corresponding to the jth eigenvalue) failed to converge. If the ith and $(i+1)$th columns of VL contain a selected complex eigenvector, then IFAILL(i) and IFAILL($i+1$) are set to the same value.

IFAILL is not referenced if JOB = 'R'.

18: IFAILR(*) — INTEGER array *Output*

Note: the dimension of the array IFAILR must be at least max(1,MM) if JOB = 'R' or 'B' and at least 1 if JOB = 'L'.

On exit: if JOB = 'R' or 'B', then IFAILR(i) = 0 if the selected right eigenvector converged and IFAILR(i) = $j > 0$ if the eigenvector stored in the ith column of VR (corresponding to the jth eigenvalue) failed to converge. If the ith and $(i+1)$th columns of VR contain a selected complex eigenvector, then IFAILR(i) and IFAILR($i+1$) are set to the same value.

IFAILR is not referenced if JOB = 'L'.

19: INFO — INTEGER *Output*

On exit: INFO = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

INFO < 0

If INFO = $-i$, the ith parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO = i, then i eigenvectors (as indicated by the parameters IFAILL and/or IFAILR above) failed to converge. The corresponding columns of VL and/or VR contain no useful information.

7 Accuracy

Each computed right eigenvector x_i is the exact eigenvector of a nearby matrix $A + E_i$, such that $\| E_i \| = O(\epsilon)\| A \|$. Hence the residual is small:

$$\| Ax_i - \lambda_i x_i \| = O(\epsilon)\| A \|.$$

However eigenvectors corresponding to close or coincident eigenvalues may not accurately span the relevant subspaces.

Similar remarks apply to computed left eigenvectors.

8 Further Comments

The complex analogue of this routine is F08PXF (CHSEIN/ZHSEIN).

9 Example

See the example for Section 9 of the document for F08NGF.