NAG Library Routine Document

F08PKF (DHSEIN)

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 (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, VL,      &
                   LDVL, VR, LDVR, MM, M, WORK, IFAILL, IFAILR, INFO)
INTEGER            N, LDH, LDVL, LDVR, MM, M, IFAILL(*), IFAILR(*),        &
                   INFO
REAL (KIND=nag_wp) H(LDH,*), WR(*), WI(*), VL(LDVL,*), VR(LDVR,*),         &
                   WORK((N+2)*N)
LOGICAL            SELECT(*)
CHARACTER(1)       JOB, EIGSRC, INITV
```

The routine may be called by its LAPACK name ***dhsein***.

3 Description

F08PKF (DHSEIN) 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:

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

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 the eigenvectors of H may be transformed to eigenvectors of A by a call to F08NGF (DORMHR).

4 References

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

5 Arguments

1: JOB – CHARACTER(1) *Input*

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

JOB = 'R'
: Only right eigenvectors are computed.

JOB = 'L'
: Only left eigenvectors are computed.

JOB = 'B'
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 (DHSEQR).

EIGSRC = 'Q'
The eigenvalues of H were found using F08PEF (DHSEQR); thus if H has any zero subdiagonal 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.

EIGSRC = 'N'
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 you are supplying initial estimates for the selected eigenvectors.

INITV = 'N'
No initial estimates are supplied.

INITV = 'U'
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 $\max(1, \mathrm{N})$.

On entry: 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 ≥ 0.

6: H(LDH, $*$) – REAL (KIND=nag_wp) array *Input*

Note: the second dimension of the array H must be at least $\max(1, \mathrm{N})$.

On entry: the n by n upper Hessenberg matrix H. If a NaN is detected in H, the routine will return with INFO $= -6$.

Constraint: No element of H is equal to NaN.

7: LDH – INTEGER *Input*

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

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

8: WR(∗) – REAL (KIND=nag_wp) array *Input/Output*
9: WI(∗) – REAL (KIND=nag_wp) array *Input*

Note: the dimension of the arrays WR and WI must be at least $\max(1, \mathrm{N})$.

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 (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 (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array VL must be at least $\max(1, \mathrm{MM})$ 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.

If JOB = 'R', VL is not referenced.

11: LDVL – INTEGER *Input*

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

Constraints:

if JOB = 'L' or 'B', LDVL $\geq$ N;
if JOB = 'R', LDVL ≥ 1.

12: VR(LDVR, ∗) – REAL (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array VR must be at least $\max(1, \mathrm{MM})$ 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.

If JOB = 'L', VR is not referenced.

13: LDVR – INTEGER *Input*

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

Constraints:

if JOB = 'R' or 'B', LDVR $\geq$ N;
if JOB = 'L', LDVR ≥ 1.

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); $0 \leq m \leq n$.

Constraint: MM $\geq m$.

15: M – INTEGER *Output*

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

16: WORK$((\mathrm{N}+2) \times \mathrm{N})$ – REAL (KIND=nag_wp) array *Workspace*

17: IFAILL$(*)$ – INTEGER array *Output*

Note: the dimension of the array IFAILL must be at least $\max(1, \mathrm{MM})$ 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 as held in $(\mathrm{WR}(j), \mathrm{WI}(j))$ 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.

If JOB = 'R', IFAILL is not referenced.

18: IFAILR$(*)$ – INTEGER array *Output*

Note: the dimension of the array IFAILR must be at least $\max(1, \mathrm{MM})$ 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 row or column of VR (corresponding to the jth eigenvalue as held in $(\mathrm{WR}(j), \mathrm{WI}(j))$) failed to converge. If the ith and $(i+1)$th rows or columns of VR contain a selected complex eigenvector, then IFAILR(i) and IFAILR$(i+1)$ are set to the same value.

If JOB = 'L', IFAILR is not referenced.

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 $= -i$, argument i 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 arguments 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 Parallelism and Performance

F08PKF (DHSEIN) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F08PKF (DHSEIN) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

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

10 Example

See Section 10 in F08NGF (DORMHR).