NAG Library Routine Document F08XEF (DHGEOZ)

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

F08XEF (DHGEQZ) implements the QZ method for finding generalized eigenvalues of the real matrix pair (A, B) of order n, which is in the generalized upper Hessenberg form.

2 Specification

```
SUBROUTINE FO8XEF (JOB, COMPQ, COMPZ, N, ILO, IHI, A, LDA, B, LDB, ALPHAR, ALPHAI, BETA, Q, LDQ, Z, LDZ, WORK, LWORK, INFO)

INTEGER

N, ILO, IHI, LDA, LDB, LDQ, LDZ, LWORK, INFO

REAL (KIND=nag_wp) A(LDA,*), B(LDB,*), ALPHAR(N), ALPHAI(N), BETA(N), Q(LDQ,*), Z(LDZ,*), WORK(max(1,LWORK))

CHARACTER(1) JOB, COMPQ, COMPZ
```

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

3 Description

F08XEF (DHGEQZ) implements a single-double-shift version of the QZ method for finding the generalized eigenvalues of the real matrix pair (A,B) which is in the generalized upper Hessenberg form. If the matrix pair (A,B) is not in the generalized upper Hessenberg form, then the routine F08WEF (DGGHRD) should be called before invoking F08XEF (DHGEQZ).

This problem is mathematically equivalent to solving the equation

$$\det(A - \lambda B) = 0.$$

Note that, to avoid underflow, overflow and other arithmetic problems, the generalized eigenvalues λ_j are never computed explicitly by this routine but defined as ratios between two computed values, α_j and β_j :

$$\lambda_i = \alpha_i / \beta_i$$
.

The parameters α_j , in general, are finite complex values and β_i are finite real non-negative values.

If desired, the matrix pair (A,B) may be reduced to generalized Schur form. That is, the transformed matrix B is upper triangular and the transformed matrix A is block upper triangular, where the diagonal blocks are either 1 by 1 or 2 by 2. The 1 by 1 blocks provide generalized eigenvalues which are real and the 2 by 2 blocks give complex generalized eigenvalues.

The parameter JOB specifies two options. If JOB = 'S' then the matrix pair (A, B) is simultaneously reduced to Schur form by applying one orthogonal transformation (usually called Q) on the left and another (usually called Z) on the right. That is,

$$A \leftarrow Q^{\mathsf{T}} A Z \\ B \leftarrow Q^{\mathsf{T}} B Z$$

The 2 by 2 upper-triangular diagonal blocks of B corresponding to 2 by 2 blocks of A will be reduced to non-negative diagonal matrices. That is, if A(j+1,j) is nonzero, then B(j+1,j) = B(j,j+1) = 0 and B(j,j) and B(j+1,j+1) will be non-negative.

If JOB = 'E', then at each iteration the same transformations are computed but they are only applied to those parts of A and B which are needed to compute α and β . This option could be used if generalized eigenvalues are required but not generalized eigenvectors.

If JOB = 'S' and COMPQ = 'V' or 'I', and COMPZ = 'V' or 'I', then the orthogonal transformations used to reduce the pair (A, B) are accumulated into the input arrays Q and Z. If generalized eigenvectors are required then JOB must be set to JOB = 'S' and if left (right) generalized eigenvectors are to be computed then COMPQ (COMPZ) must be set to COMPQ = 'V' or 'I' and not $COMPQ \neq 'N'$.

If COMPQ = 'I', then eigenvectors are accumulated on the identity matrix and on exit the array Q contains the left eigenvector matrix Q. However, if COMPQ = 'V' then the transformations are accumulated on the user-supplied matrix Q_0 in array Q on entry and thus on exit Q contains the matrix product QQ_0 . A similar convention is used for COMPZ.

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

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

Moler C B and Stewart G W (1973) An algorithm for generalized matrix eigenproblems SIAM J. Numer. Anal. 10 241–256

Stewart G W and Sun J-G (1990) Matrix Perturbation Theory Academic Press, London

5 Parameters

1: JOB – CHARACTER(1)

Input

On entry: specifies the operations to be performed on (A, B).

JOB = 'E'

The matrix pair (A, B) on exit might not be in the generalized Schur form.

JOB = 'S'

The matrix pair (A, B) on exit will be in the generalized Schur form.

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

2: COMPQ - CHARACTER(1)

Input

On entry: specifies the operations to be performed on Q:

COMPQ = 'N'

The array Q is unchanged.

COMPO = 'V'

The left transformation Q is accumulated on the array Q.

COMPO = 'I'

The array Q is initialized to the identity matrix before the left transformation Q is accumulated in Q.

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

3: COMPZ – CHARACTER(1)

Input

On entry: specifies the operations to be performed on Z.

COMPZ = 'N'

The array Z is unchanged.

COMPZ = 'V'

The right transformation Z is accumulated on the array Z.

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COMPZ = 'I'

The array Z is initialized to the identity matrix before the right transformation Z is accumulated in Z.

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

4: N - INTEGER Input

On entry: n, the order of the matrices A, B, Q and Z.

Constraint: $N \ge 0$.

5: ILO – INTEGER
 6: IHI – INTEGER
 Input

On entry: the indices i_{lo} and i_{hi} , respectively which define the upper triangular parts of A. The submatrices $A(1:i_{lo}-1,1:i_{lo}-1)$ and $A(i_{hi}+1:n,i_{hi}+1:n)$ are then upper triangular. These parameters are provided by F08WHF (DGGBAL) if the matrix pair was previously balanced; otherwise, ILO = 1 and IHI = N.

Constraints:

if
$$N > 0$$
, $1 \le ILO \le IHI \le N$;
if $N = 0$, $ILO = 1$ and $IHI = 0$.

7: A(LDA,*) - REAL (KIND=nag_wp) array Input/Output

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

On entry: the n by n upper Hessenberg matrix A. The elements below the first subdiagonal must be set to zero.

On exit: if JOB = 'S', the matrix pair (A, B) will be simultaneously reduced to generalized Schur form.

If JOB = 'E', the 1 by 1 and 2 by 2 diagonal blocks of the matrix pair (A, B) will give generalized eigenvalues but the remaining elements will be irrelevant.

8: LDA – INTEGER Input

On entry: the first dimension of the array A as declared in the (sub)program from which F08XEF (DHGEQZ) is called.

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

9: B(LDB,*) - REAL (KIND=nag_wp) array Input/Output

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

On entry: the n by n upper triangular matrix B. The elements below the diagonal must be zero.

On exit: if JOB = 'S', the matrix pair (A, B) will be simultaneously reduced to generalized Schur form.

If JOB = 'E', the 1 by 1 and 2 by 2 diagonal blocks of the matrix pair (A, B) will give generalized eigenvalues but the remaining elements will be irrelevant.

10: LDB – INTEGER Input

On entry: the first dimension of the array B as declared in the (sub)program from which F08XEF (DHGEQZ) is called.

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

11: ALPHAR(N) – REAL (KIND=nag_wp) array Output

On exit: the real parts of α_j , for j = 1, 2, ..., n.

12: ALPHAI(N) - REAL (KIND=nag_wp) array

Output

On exit: the imaginary parts of α_j , for j = 1, 2, ..., n.

13: BETA(N) – REAL (KIND=nag_wp) array

Output

On exit: β_i , for $j = 1, 2, \dots, n$.

14: Q(LDQ,*) - REAL (KIND=nag wp) array

Input/Output

Note: the second dimension of the array Q must be at least max(1, N) if COMPQ = 'V' or 'I' and at least 1 if COMPQ = 'N'.

On entry: if COMPQ = 'V', the matrix Q_0 . The matrix Q_0 is usually the matrix Q returned by F08WEF (DGGHRD).

If COMPQ = 'N', Q is not referenced.

On exit: if COMPQ = 'V', Q contains the matrix product QQ_0 .

If COMPQ = I', Q contains the transformation matrix Q.

15: LDQ – INTEGER

Input

On entry: the first dimension of the array Q as declared in the (sub)program from which F08XEF (DHGEQZ) is called.

Constraints:

if
$$COMPQ = 'V'$$
 or 'I', $LDQ \ge N$; if $COMPQ = 'N'$, $LDQ \ge 1$.

16: Z(LDZ,*) - REAL (KIND=nag wp) array

Input/Output

Note: the second dimension of the array Z must be at least max(1, N) if COMPZ = 'V' or 'I' and at least 1 if COMPZ = 'N'.

On entry: if COMPZ = 'V', the matrix Z_0 . The matrix Z_0 is usually the matrix Z returned by F08WEF (DGGHRD).

If COMPZ = 'N', Z is not referenced.

On exit: if COMPZ = 'V', Z contains the matrix product ZZ_0 .

If COMPZ = 'I', Z contains the transformation matrix Z.

17: LDZ – INTEGER

Input

On entry: the first dimension of the array Z as declared in the (sub)program from which F08XEF (DHGEQZ) is called.

Constraints:

if
$$COMPZ = 'V'$$
 or 'I', $LDZ \ge N$; if $COMPZ = 'N'$, $LDZ > 1$.

18: WORK(max(1,LWORK)) - REAL (KIND=nag wp) array

Workspace

On exit: if INFO = 0, WORK(1) contains the minimum value of LWORK required for optimal performance.

19: LWORK – INTEGER

Input

On entry: the dimension of the array WORK as declared in the (sub)program from which F08XEF (DHGEQZ) is called.

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If LWORK = -1, a workspace query is assumed; the routine only calculates the minimum size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

Constraint: LWORK $\geq \max(1, N)$ or LWORK = -1.

20: INFO – INTEGER Output

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

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

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 $1 \le \text{INFO} \le \text{N}$, the QZ iteration did not converge and the matrix pair (A, B) is not in the generalized Schur form at exit. However, if INFO < N, then the computed α_i and β_i should be correct for $i = \text{INFO} + 1, \dots, \text{N}$.

If $N+1 \le INFO \le 2 \times N$, the computation of shifts failed and the matrix pair (A,B) is not in the generalized Schur form at exit. However, if $INFO < 2 \times N$, then the computed α_i and β_i should be correct for i = INFO - N + 1, ..., N.

If INFO $> 2 \times N$, then an unexpected Library error has occurred. Please contact NAG with details of your program.

7 Accuracy

Please consult Section 4.11 of the LAPACK Users' Guide (see Anderson et al. (1999)) and Chapter 6 of Stewart and Sun (1990), for more information.

8 Further Comments

F08XEF (DHGEQZ) is the fifth step in the solution of the real generalized eigenvalue problem and is called after F08WEF (DGGHRD).

The complex analogue of this routine is F08XSF (ZHGEQZ).

9 Example

This example computes the α and β parameters, which defines the generalized eigenvalues, of the matrix pair (A, B) given by

$$A = \begin{pmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 2.0 & 4.0 & 8.0 & 16.0 & 32.0 \\ 3.0 & 9.0 & 27.0 & 81.0 & 243.0 \\ 4.0 & 16.0 & 64.0 & 256.0 & 1024.0 \\ 5.0 & 25.0 & 125.0 & 625.0 & 3125.0 \end{pmatrix}$$

$$B = \begin{pmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ 1.0 & 4.0 & 9.0 & 16.0 & 25.0 \\ 1.0 & 8.0 & 27.0 & 64.0 & 125.0 \\ 1.0 & 16.0 & 81.0 & 256.0 & 625.0 \\ 1.0 & 32.0 & 243.0 & 1024.0 & 3125.0 \end{pmatrix}.$$

This requires calls to five routines: F08WHF (DGGBAL) to balance the matrix, F08AEF (DGEQRF) to perform the QR factorization of B, F08AGF (DORMQR) to apply Q to A, F08WEF (DGGHRD) to reduce the matrix pair to the generalized Hessenberg form and F08XEF (DHGEQZ) to compute the eigenvalues using the QZ algorithm.

9.1 Program Text

```
Program f08xefe
      FO8XEF Example Program Text
     Mark 24 Release. NAG Copyright 2012.
!
      .. Use Statements ..
     Use nag_library, Only: dgeqrf, dggbal, dgghrd, dhgeqz, dormqr, nag_wp,
                             x04caf
!
      .. Implicit None Statement ..
     Implicit None
1
      .. Parameters ..
      Integer, Parameter
                                       :: nin = 5, nout = 6
!
      .. Local Scalars ..
                                        :: i, ifail, ihi, ilo, info, irows,
     Integer
                                           jwork, lda, ldb, ldq, ldz, lwork, n
     Character (1)
                                        :: compq, compz, job
      .. Local Arrays ..
     Real (Kind=nag_wp), Allocatable
                                       :: a(:,:), alphai(:), alphar(:),
                                           b(:,:), beta(:), lscale(:), q(:,:),
                                           rscale(:), tau(:), work(:), z(:,:)
!
      .. Intrinsic Procedures ..
     Intrinsic
                                        :: nint
      .. Executable Statements ..
!
      Write (nout,*) 'FO8XEF Example Program Results'
     Flush (nout)
     Skip heading in data file
1
     Read (nin,*)
     Read (nin,*) n
      ldq = 1
      ldz = 1
      lda = n
      ldb = n
      lwork = 6*n
     Allocate (alphai(n),alphar(n),beta(n),a(lda,n),lscale(n),q(ldq,ldq), &
       rscale(n),b(ldb,n),tau(n),work(lwork),z(ldz,ldz))
     READ matrix A from data file
     Read (nin,*)(a(i,1:n),i=1,n)
     READ matrix B from data file
     Read (nin,*)(b(i,1:n),i=1,n)
     Balance matrix pair (A,B)
!
      job = 'B'
      The NAG name equivalent of dggbal is f08whf
     Call dggbal(job,n,a,lda,b,ldb,ilo,ihi,lscale,rscale,work,info)
!
     Matrix A after balancing
!
      ifail: behaviour on error exit
              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
!
      ifail = 0
     Call x04caf('General',' ',n,n,a,lda,'Matrix A after balancing',ifail)
     Write (nout,*)
     Flush (nout)
     Matrix B after balancing
```

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```
ifail = 0
      Call x04caf('General',' ',n,n,b,ldb,'Matrix B after balancing',ifail)
     Write (nout,*)
     Flush (nout)
     Reduce B to triangular form using QR
      irows = ihi + 1 - ilo
     The NAG name equivalent of dgeqrf is f08aef
!
      Call dgeqrf(irows,irows,b(ilo,ilo),ldb,tau,work,lwork,info)
      Apply the orthogonal transformation to matrix A
      The NAG name equivalent of dormqr is f08agf
      Call dormqr('L','T',irows,irows,irows,b(ilo,ilo),ldb,tau,a(ilo,ilo),lda, &
        work, lwork, info)
1
      Compute the generalized Hessenberg form of (A,B) -> (H,T)
      compq = 'N'
      comp\bar{z} = 'N'
      The NAG name equivalent of dgghrd is f08wef
!
      Call dgghrd(compq,compz,irows,1,irows,a(ilo,ilo),lda,b(ilo,ilo),ldb,q, &
        ldq,z,ldz,info)
     Matrix A (H) in generalized Hessenberg form.
!
      ifail = 0
      Call x04caf('General',' ',n,n,a,lda,'Matrix A in Hessenberg form',ifail)
     Write (nout,*)
     Flush (nout)
     Matrix B (T) in generalized Hessenberg form.
      ifail = 0
     Call x04caf('General',' ',n,n,b,ldb,'Matrix B is triangular',ifail)
     Routine DHGEQZ
1
     Workspace query: jwork = -1
      jwork = -1
      job = 'E'
      The NAG name equivalent of dhgeqz is f08xef
!
      Call dhgeqz(job,compq,compz,n,ilo,ihi,a,lda,b,ldb,alphar,alphai,beta,q, &
        ldq,z,ldz,work,jwork,info)
     Write (nout,*)
      Write (nout,99999) nint(work(1))
     Write (nout,99998) lwork
     Write (nout, *)
      Compute the generalized Schur form
      if the workspace lwork is adequate
      If (nint(work(1)) <= lwork) Then</pre>
        The NAG name equivalent of dhgeqz is f08xef
!
        Call dhgeqz(job,compq,compz,n,ilo,ihi,a,lda,b,ldb,alphar,alphai,beta, &
          q,ldq,z,ldz,work,lwork,info)
        Print the generalized eigenvalues
!
        Write (nout, 99997)
        Do i = 1, n
          If (beta(i)/=0.0E0_nag_wp) Then
            Write (nout,99996) i, '(', alphar(i)/beta(i), ',', &
    alphai(i)/beta(i), ')'
```

```
Else
Write (nout,99994) i
End If
End Do
Else
Write (nout,99995)
End If

99999 Format (1X,'Minimal required LWORK = ',I6)
99998 Format (1X,'Actual value of LWORK = ',I6)
99997 Format (1X,'Generalized eigenvalues')
99996 Format (1X,I4,5X,A,F7.3,A,F7.3,A)
99995 Format (1X,Insufficient workspace allocated for call to FO8XEF/DHGEQZ')
99994 Format (1X,I4,'Eigenvalue is infinite')
End Program fO8xefe
```

9.2 Program Data

F08XEF Example Program Data							
5					:Value of N		
1.00	1.00	1.00	1.00	1.00			
2.00	4.00	8.00	16.00	32.00			
3.00	9.00	27.00	81.00	243.00			
4.00	16.00	64.00	256.00	1024.00			
5.00	25.00	125.00	625.00	3125.00	:End of matrix A		
1.00	2.00	3.00	4.00	5.00			
1.00	4.00	9.00	16.00	25.00			
1.00	8.00	27.00	64.00	125.00			
1.00	16.00	81.00	256.00	625.00			
1.00	32.00	243.00	1024.00	3125.00	:End of matrix B		

9.3 Program Results

		Program Res	ults					
Matrix	A after 1	_	_		_			
_	1	2	3	4	5			
1	1.0000	1.0000	0.1000	0.1000	0.1000			
2	2.0000	4.0000	0.8000	1.6000	3.2000			
3	0.3000	0.9000	0.2700	0.8100	2.4300			
4	0.4000	1.6000	0.6400	2.5600	10.2400			
5	0.5000	2.5000	1.2500	6.2500	31.2500			
Matrix	B after l	balancing						
	1	2	3	4	5			
1	1.0000	2.0000	0.3000	0.4000	0.5000			
2	1.0000	4.0000	0.9000	1.6000	2.5000			
3	0.1000	0.8000	0.2700	0.6400	1.2500			
4	0.1000	1.6000	0.8100	2.5600	6.2500			
5	0.1000	3.2000	2.4300	10.2400	31.2500			
Matrix	A in Hes	senberg for	m					
	1	2	3	4	5			
1	-2.1898	-0.3181	2.0547	4.7371	-4.6249			
	-0.8395	-0.0426	1.7132	7.5194	- 17.1850			
3	0.0000	-0.2846	-1.0101	- 7.5927	26.4499			
4	0.0000	0.0000	0.0376	1.4070	-3.3643			
5	0.0000	0.0000	0.0000	0.3813	-0.9937			
Matrix B is triangular								
	1	2	3	4	5			
1	-1.4248	-0.3476	2.1175	5.5813	-3.9269			
2	0.0000	-0.0782	0.1189	8.0940	- 15.2928			
3	0.0000	0.0000	1.0021	-10.9356	26.5971			
4	0.0000	0.0000	0.0000	0.5820	-0.0730			
5	0.0000	0.0000	0.0000	0.0000	0.5321			
Minima	l require	d LWORK =	5					
	value of	LWORK =	30					

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Generali	zed	eigenvalues		
1	(·	-2.437,	0.000)	
2	(0.607,	0.795)	
3	(0.607,	-0.795)	
4	(1.000,	0.000)	
5	(·	-0.410,	0.000)	

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