

NAG Library Routine Document

F08SSF (ZHEGST)

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

F08SSF (ZHEGST) reduces a complex Hermitian-definite generalized eigenproblem $Az = \lambda Bz$, $ABz = \lambda z$ or $BAz = \lambda z$ to the standard form $Cy = \lambda y$, where A is a complex Hermitian matrix and B has been factorized by F07FRF (ZPOTRF).

2 Specification

```
SUBROUTINE F08SSF (ITYPE, UPLO, N, A, LDA, B, LDB, INFO)
  INTEGER          ITYPE, N, LDA, LDB, INFO
  COMPLEX (KIND=nag_wp) A(LDA,*), B(LDB,*)
  CHARACTER(1)    UPLO
```

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

3 Description

To reduce the complex Hermitian-definite generalized eigenproblem $Az = \lambda Bz$, $ABz = \lambda z$ or $BAz = \lambda z$ to the standard form $Cy = \lambda y$, F08SSF (ZHEGST) must be preceded by a call to F07FRF (ZPOTRF) which computes the Cholesky factorization of B ; B must be positive definite.

The different problem types are specified by the argument ITYPE, as indicated in the table below. The table shows how C is computed by the routine, and also how the eigenvectors z of the original problem can be recovered from the eigenvectors of the standard form.

ITYPE	Problem	UPLO	B	C	z
1	$Az = \lambda Bz$	'U' 'L'	$U^H U$ LL^H	$U^{-H} A U^{-1}$ $L^{-1} A L^{-H}$	$U^{-1} y$ $L^{-H} y$
2	$ABz = \lambda z$	'U' 'L'	$U^H U$ LL^H	$U A U^H$ $L^H A L$	$U^{-1} y$ $L^{-H} y$
3	$BAz = \lambda z$	'U' 'L'	$U^H U$ LL^H	$U A U^H$ $L^H A L$	$U^H y$ $L y$

4 References

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

5 Arguments

- 1: ITYPE – INTEGER *Input*
On entry: indicates how the standard form is computed.
 ITYPE = 1
 if UPLO = 'U', $C = U^{-H}AU^{-1}$;
 if UPLO = 'L', $C = L^{-1}AL^{-H}$.
 ITYPE = 2 or 3
 if UPLO = 'U', $C = UAU^H$;
 if UPLO = 'L', $C = L^HAL$.
Constraint: ITYPE = 1, 2 or 3.
- 2: UPLO – CHARACTER(1) *Input*
On entry: indicates whether the upper or lower triangular part of A is stored and how B has been factorized.
 UPLO = 'U'
 The upper triangular part of A is stored and $B = U^HU$.
 UPLO = 'L'
 The lower triangular part of A is stored and $B = LL^H$.
Constraint: UPLO = 'U' or 'L'.
- 3: N – INTEGER *Input*
On entry: n , the order of the matrices A and B .
Constraint: $N \geq 0$.
- 4: A(LDA,*) – COMPLEX (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 Hermitian matrix A .
 If UPLO = 'U', the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.
 If UPLO = 'L', the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.
On exit: the upper or lower triangle of A is overwritten by the corresponding upper or lower triangle of C as specified by ITYPE and UPLO.
- 5: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F08SSF (ZHEGST) is called.
Constraint: $LDA \geq \max(1, N)$.
- 6: B(LDB,*) – COMPLEX (KIND=nag_wp) array *Input*
Note: the second dimension of the array B must be at least $\max(1, N)$.
On entry: the Cholesky factor of B as specified by UPLO and returned by F07FRF (ZPOTRF).

7: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F08SSF (ZHEGST) is called.

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

8: 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.

7 Accuracy

Forming the reduced matrix C is a stable procedure. However it involves implicit multiplication by B^{-1} (if ITYPE = 1) or B (if ITYPE = 2 or 3). When F08SSF (ZHEGST) is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if B is ill-conditioned with respect to inversion. See the document for F08SNF (ZHEGV) for further details.

8 Parallelism and Performance

F08SSF (ZHEGST) 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 total number of real floating-point operations is approximately $4n^3$.

The real analogue of this routine is F08SEF (DSYGST).

10 Example

This example computes all the eigenvalues of $Az = \lambda Bz$, where

$$A = \begin{pmatrix} -7.36 + 0.00i & 0.77 - 0.43i & -0.64 - 0.92i & 3.01 - 6.97i \\ 0.77 + 0.43i & 3.49 + 0.00i & 2.19 + 4.45i & 1.90 + 3.73i \\ -0.64 + 0.92i & 2.19 - 4.45i & 0.12 + 0.00i & 2.88 - 3.17i \\ 3.01 + 6.97i & 1.90 - 3.73i & 2.88 + 3.17i & -2.54 + 0.00i \end{pmatrix}$$

and

$$B = \begin{pmatrix} 3.23 + 0.00i & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 + 0.00i & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 + 0.00i & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 + 0.00i \end{pmatrix}.$$

Here B is Hermitian positive definite and must first be factorized by F07FRF (ZPOTRF). The program calls F08SSF (ZHEGST) to reduce the problem to the standard form $Cy = \lambda y$; then F08FSF (ZHETRD) to reduce C to tridiagonal form, and F08JFF (DSTERF) to compute the eigenvalues.

10.1 Program Text

```

Program f08ssf

!      F08SSF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
Use nag_library, Only: dsterf, nag_wp, zhegst, zhetrd, zpotrf
!      .. Implicit None Statement ..
Implicit None
!      .. Parameters ..
Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
Integer                    :: i, info, lda, ldb, lwork, n
Character (1)              :: uplo
!      .. Local Arrays ..
Complex (Kind=nag_wp), Allocatable :: a(:,,:), b(:,,:), tau(:), work(:)
Real (Kind=nag_wp), Allocatable  :: d(:), e(:)
!      .. Executable Statements ..
Write (nout,*) 'F08SSF Example Program Results'
!      Skip heading in data file
Read (nin,*)
Read (nin,*) n
lda = n
ldb = n
lwork = 64*n
Allocate (a(lda,n),b(ldb,n),tau(n),work(lwork),d(n),e(n-1))

!      Read A and B from data file

Read (nin,*) uplo
If (uplo=='U') Then
  Read (nin,*)(a(i,i:n),i=1,n)
  Read (nin,*)(b(i,i:n),i=1,n)
Else If (uplo=='L') Then
  Read (nin,*)(a(i,1:i),i=1,n)
  Read (nin,*)(b(i,1:i),i=1,n)
End If

!      Compute the Cholesky factorization of B
!      The NAG name equivalent of zpotrf is f07frf
Call zpotrf(uplo,n,b,ldb,info)

Write (nout,*)
If (info>0) Then
  Write (nout,*) 'B is not positive definite.'
Else

!      Reduce the problem to standard form C*y = lambda*y, storing
!      the result in A
!      The NAG name equivalent of zhegst is f08ssf
Call zhegst(1,uplo,n,a,lda,b,ldb,info)

!      Reduce C to tridiagonal form T = (Q**H)*C*Q
!      The NAG name equivalent of zhetrd is f08fsf
Call zhetrd(uplo,n,a,lda,d,e,tau,work,lwork,info)

!      Calculate the eigenvalues of T (same as C)
!      The NAG name equivalent of dsterf is f08jff
Call dsterf(n,d,e,info)

If (info>0) Then
  Write (nout,*) 'Failure to converge.'
Else

!      Print eigenvalues

Write (nout,*) 'Eigenvalues'
Write (nout,99999) d(1:n)

```

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      End If
    End If

99999 Format (3X,(9F8.4))
      End Program f08ssfe

```

10.2 Program Data

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F08SSF Example Program Data
  4                                     :Value of N
  'L'                                 :Value of UPLO
(-7.36, 0.00)
( 0.77, 0.43) ( 3.49, 0.00)
(-0.64, 0.92) ( 2.19,-4.45) ( 0.12, 0.00)
( 3.01, 6.97) ( 1.90,-3.73) ( 2.88, 3.17) (-2.54, 0.00) :End of matrix A
( 3.23, 0.00)
( 1.51, 1.92) ( 3.58, 0.00)
( 1.90,-0.84) (-0.23,-1.11) ( 4.09, 0.00)
( 0.42,-2.50) (-1.18,-1.37) ( 2.33, 0.14) ( 4.29, 0.00) :End of matrix B

```

10.3 Program Results

F08SSF Example Program Results

```

Eigenvalues
-5.9990 -2.9936  0.5047  3.9990

```
