NAG Fortran Library Routine Document F08TSF (ZHPGST)

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

F08TSF (ZHPGST) 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 F07GRF (ZPPTRF), using packed storage.

2 Specification

```
SUBROUTINE FO8TSF (ITYPE, UPLO, N, AP, BP, INFO)

INTEGER ITYPE, N, INFO

complex*16 AP(*), BP(*)

CHARACTER*1 UPLO
```

The routine may be called by its LAPACK name zhpgst.

3 Description

To reduce the complex Hermitian-definite generalized eigenproblem $Az = \lambda Bz$, $ABz = \lambda z$ or $BAz = \lambda z$ to the standard form $Cy = \lambda y$ using packed storage, F08TSF (ZHPGST) must be preceded by a call to F07GRF (ZPPTRF) which computes the Cholesky factorization of B; B must be positive-definite.

The different problem types are specified by the parameter 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	В	С	Z
1	$Az = \lambda Bz$	'U' 'L'	$U^{ m H}U$ $LL^{ m H}$	$U^{-\mathrm{H}}AU^{-1}$ $L^{-1}AL^{-\mathrm{H}}$	$U^{-1}y$ $L^{-H}y$
2	$ABz = \lambda z$	'U' 'L'	$U^{\mathrm{H}}U$ LL^{H}	$UAU^{ m H} \ L^{ m H}AL$	$U^{-1}y$ $L^{-H}y$
3	$BAz = \lambda z$	'U' 'L'	$U^{\mathrm{H}}U$ LL^{H}	$UAU^{ m H} \ L^{ m H}AL$	U ^H y Ly

4 References

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

5 Parameters

1: ITYPE – INTEGER Input

On entry: indicates how the standard form is computed.

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$$\begin{split} \text{ITYPE} &= 1 \\ &\text{if UPLO} = \text{'U'}, \ C = U^{-\text{H}}AU^{-1}; \\ &\text{if UPLO} = \text{'L'}, \ C = L^{-1}AL^{-\text{H}}. \\ \\ \text{ITYPE} &= 2 \text{ or } 3 \\ &\text{if UPLO} = \text{'U'}, \ C = UAU^{\text{H}}; \\ &\text{if UPLO} = \text{'L'}, \ C = L^{\text{H}}AL. \end{split}$$

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 $B = U^{H}U$.

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: AP(*) - complex*16 array

Input/Output

Note: the dimension of the array AP must be at least $max(1, N \times (N+1)/2)$.

On entry: the n by n Hermitian matrix A, packed by columns. More precisely,

if UPLO = 'U', the upper triangular part of A must be stored with element a_{ij} in AP(i+j(j-1)/2) for $i \le j$;

if UPLO = 'L', the lower triangular part of A must be stored with element a_{ij} in AP(i + (2n - j)(j - 1)/2) for $i \ge j$.

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, using the same packed storage format as described above.

5: BP(*) - complex*16 array

Input

Note: the dimension of the array BP must be at least $max(1, N \times (N+1)/2)$.

On entry: the Cholesky factor of B as specified by UPLO and returned by F07GRF (ZPPTRF).

6: 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, the *i*th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

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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 F08TSF (ZHPGST) 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 Further Comments

The total number of real floating-point operations is approximately $4n^3$.

The real analogue of this routine is F08TEF (DSPGST).

9 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

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

using packed storage. Here B is Hermitian positive-definite and must first be factorized by F07GRF (ZPPTRF). The program calls F08TSF (ZHPGST) to reduce the problem to the standard form $Cy = \lambda y$; then F08GSF (ZHPTRD) to reduce C to tridiagonal form, and F08JFF (DSTERF) to compute the eigenvalues.

9.1 Program Text

```
FO8TSF Example Program Text
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.. Parameters ..
INTEGER
                NIN, NOUT
PARAMETER
                (NIN=5, NOUT=6)
                NMAX
INTEGER
PARAMETER
                (NMAX=8)
.. Local Scalars ..
INTEGER I, INFO, J, N
CHARACTER
                UPLO
.. Local Arrays ..
COMPLEX *16 AP(NMAX*(NMAX+1)/2), BP(NMAX*(NMAX+1)/2),
                TAU(NMAX)
DOUBLE PRECISION D(NMAX), E(NMAX-1)
.. External Subroutines ..
EXTERNAL DSTERF, ZHPGST, ZHPTRD, ZPPTRF
.. Executable Statements ..
WRITE (NOUT,*) 'FO8TSF Example Program Results'
Skip heading in data file
READ (NIN, *)
READ (NIN,*) N
IF (N.LE.NMAX) THEN
   Read A and B from data file
   READ (NIN,*) UPLO
   IF (UPLO.EQ.'U') THEN
      READ (NIN,*) ((AP(I+J*(J-1)/2),J=I,N),I=1,N)
      READ (NIN, *) ((BP(I+J*(J-1)/2), J=I, N), I=1, N)
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ELSE IF (UPLO.EQ.'L') THEN
            READ (NIN,*) ((AP(I+(2*N-J)*(J-1)/2),J=1,I),I=1,N)
            READ (NIN,*) ((BP(I+(2*N-J)*(J-1)/2),J=1,I),I=1,N)
         END IF
         Compute the Cholesky factorization of B
         CALL ZPPTRF(UPLO,N,BP,INFO)
         WRITE (NOUT,*)
         IF (INFO.GT.O) THEN
            WRITE (NOUT, *) 'B is not positive-definite.'
            Reduce the problem to standard form C*y = lambda*y, storing
            the result in A
            CALL ZHPGST(1,UPLO,N,AP,BP,INFO)
            Reduce C to tridiagonal form T = (Q**H)*C*Q
            CALL ZHPTRD (UPLO, N, AP, D, E, TAU, INFO)
            Calculate the eigenvalues of T (same as C)
            CALL DSTERF (N,D,E,INFO)
            IF (INFO.GT.O) THEN
              WRITE (NOUT,*) 'Failure to converge.'
            ELSE
               Print eigenvalues
               WRITE (NOUT,*) 'Eigenvalues'
               WRITE (NOUT, 99999) (D(I), I=1, N)
            END IF
        END IF
     END IF
      STOP
99999 FORMAT (3X, (9F8.4))
     END
```

9.2 Program Data

```
FO8TSF Example Program Data

4
'L'
(-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
```

9.3 Program Results

```
FO8TSF Example Program Results

Eigenvalues
-5.9990 -2.9936 0.5047 3.9990
```