NAG Library Routine Document

F08UEF (DSBGST)

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

F08UEF (DSBGST) reduces a real symmetric-definite generalized eigenproblem $Az = \lambda Bz$ to the standard form $Cy = \lambda y$, where A and B are band matrices, A is a real symmetric matrix, and B has been factorized by F08UFF (DPBSTF).

2 Specification

```
SUBROUTINE F08UEF (VECT, UPLO, N, KA, KB, AB, LDAB, BB, LDBB, X, LDX,      &
                   WORK, INFO)

INTEGER             N, KA, KB, LDAB, LDBB, LDX, INFO
REAL (KIND=nag_wp) AB(LDAB,*), BB(LDBB,*), X(LDX,*), WORK(2*N)
CHARACTER(1)        VECT, UPLO
```

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

3 Description

To reduce the real symmetric-definite generalized eigenproblem $Az = \lambda Bz$ to the standard form $Cy = \lambda y$, where A, B and C are banded, F08UEF (DSBGST) must be preceded by a call to F08UFF (DPBSTF) which computes the split Cholesky factorization of the positive definite matrix B: $B = S^{\mathrm{T}}S$. The split Cholesky factorization, compared with the ordinary Cholesky factorization, allows the work to be approximately halved.

This routine overwrites A with $C = X^{\mathrm{T}}AX$, where $X = S^{-1}Q$ and Q is a orthogonal matrix chosen (implicitly) to preserve the bandwidth of A. The routine also has an option to allow the accumulation of X, and then, if z is an eigenvector of C, Xz is an eigenvector of the original system.

4 References

Crawford C R (1973) Reduction of a band-symmetric generalized eigenvalue problem *Comm. ACM* **16** 41–44

Kaufman L (1984) Banded eigenvalue solvers on vector machines *ACM Trans. Math. Software* **10** 73–86

5 Arguments

1: VECT – CHARACTER(1) *Input*

On entry: indicates whether X is to be returned.

VECT = 'N'
: X is not returned.

VECT = 'V'
: X is returned.

Constraint: VECT = 'N' or 'V'.

2: UPLO – CHARACTER(1) *Input*

On entry: indicates whether the upper or lower triangular part of A is stored.

UPLO = 'U'
: The upper triangular part of A is stored.

UPLO = 'L'
: The lower triangular part of A is stored.

Constraint: UPLO = 'U' or 'L'.

3: N – INTEGER *Input*

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

Constraint: $\text{N} \geq 0$.

4: KA – INTEGER *Input*

On entry: if UPLO = 'U', the number of superdiagonals, k_a, of the matrix A.

If UPLO = 'L', the number of subdiagonals, k_a, of the matrix A.

Constraint: $\text{KA} \geq 0$.

5: KB – INTEGER *Input*

On entry: if UPLO = 'U', the number of superdiagonals, k_b, of the matrix B.

If UPLO = 'L', the number of subdiagonals, k_b, of the matrix B.

Constraint: $\text{KA} \geq \text{KB} \geq 0$.

6: AB(LDAB, $*$) – REAL (KIND=nag_wp) array *Input/Output*

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

On entry: the upper or lower triangle of the n by n symmetric band matrix A.

The matrix is stored in rows 1 to $k_a + 1$, more precisely,

if UPLO = 'U', the elements of the upper triangle of A within the band must be stored with element A_{ij} in $\text{AB}(k_a + 1 + i - j, j)$ for $\max(1, j - k_a) \leq i \leq j$;

if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element A_{ij} in $\text{AB}(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_a)$.

On exit: the upper or lower triangle of AB is overwritten by the corresponding upper or lower triangle of C as specified by UPLO.

7: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F08UEF (DSBGST) is called.

Constraint: $\text{LDAB} \geq \text{KA} + 1$.

8: BB(LDBB, $*$) – REAL (KIND=nag_wp) array *Input*

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

On entry: the banded split Cholesky factor of B as specified by UPLO, N and KB and returned by F08UFF (DPBSTF).

9: LDBB – INTEGER *Input*

On entry: the first dimension of the array BB as declared in the (sub)program from which F08UEF (DSBGST) is called.

Constraint: $\text{LDBB} \geq \text{KB} + 1$.

10: X(LDX, $*$) – REAL (KIND=nag_wp) array *Output*

Note: the second dimension of the array X must be at least $\max(1, \text{N})$ if VECT = 'V' and at least 1 if VECT = 'N'.

On exit: the n by n matrix $X = S^{-1}Q$, if VECT = 'V'.

If VECT = 'N', X is not referenced.

11: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which F08UEF (DSBGST) is called.

Constraints:

if VECT = 'V', $\text{LDX} \geq \max(1, \text{N})$;
if VECT = 'N', $\text{LDX} \geq 1$.

12: WORK($2 \times \text{N}$) – REAL (KIND=nag_wp) array *Workspace*

13: 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}. When F08UEF (DSBGST) 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.

8 Parallelism and Performance

F08UEF (DSBGST) 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 floating-point operations is approximately $6n^2k_B$, when VECT = 'N', assuming $n \gg k_A, k_B$; there are an additional $(3/2)n^3(k_B/k_A)$ operations when VECT = 'V'.

The complex analogue of this routine is F08USF (ZHBGST).

10 Example

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

$$A = \begin{pmatrix} 0.24 & 0.39 & 0.42 & 0.00 \\ 0.39 & -0.11 & 0.79 & 0.63 \\ 0.42 & 0.79 & -0.25 & 0.48 \\ 0.00 & 0.63 & 0.48 & -0.03 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2.07 & 0.95 & 0.00 & 0.00 \\ 0.95 & 1.69 & -0.29 & 0.00 \\ 0.00 & -0.29 & 0.65 & -0.33 \\ 0.00 & 0.00 & -0.33 & 1.17 \end{pmatrix}.$$

Here A is symmetric, B is symmetric positive definite, and A and B are treated as band matrices. B must first be factorized by F08UFF (DPBSTF). The program calls F08UEF (DSBGST) to reduce the problem to the standard form $Cy = \lambda y$, then F08HEF (DSBTRD) to reduce C to tridiagonal form, and F08JFF (DSTERF) to compute the eigenvalues.

10.1 Program Text

```
    Program f08uefe

!     F08UEF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: dpbstf, dsbgst, dsbtrd, dsterf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Integer                          :: i, info, j, ka, kb, ldab, ldbb, ldx, &
                                          n
      Character (1)                    :: uplo
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: ab(:,:), bb(:,:), d(:), e(:),        &
                                          work(:), x(:,:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max, min
!     .. Executable Statements ..
      Write (nout,*) 'F08UEF Example Program Results'
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, ka, kb
      ldab = ka + 1
      ldbb = kb + 1
      ldx = n
      Allocate (ab(ldab,n),bb(ldbb,n),d(n),e(n-1),work(2*n),x(ldx,n))

!     Read A and B from data file

      Read (nin,*) uplo
      If (uplo=='U') Then
        Do i = 1, n
          Read (nin,*)(ab(ka+1+i-j,j),j=i,min(n,i+ka))
        End Do
        Do i = 1, n
          Read (nin,*)(bb(kb+1+i-j,j),j=i,min(n,i+kb))
        End Do
      Else If (uplo=='L') Then
        Do i = 1, n
          Read (nin,*)(ab(1+i-j,j),j=max(1,i-ka),i)
        End Do
        Do i = 1, n
          Read (nin,*)(bb(1+i-j,j),j=max(1,i-kb),i)
        End Do
      End If

!     Compute the split Cholesky factorization of B
!     The NAG name equivalent of dpbstf is f08uff
      Call dpbstf(uplo,n,kb,bb,ldbb,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 dsbgst is f08uef
        Call dsbgst('N',uplo,n,ka,kb,ab,ldab,bb,ldbb,x,ldx,work,info)

!       Reduce C to tridiagonal form T = (Q**T)*C*Q
!       The NAG name equivalent of dsbtrd is f08hef
        Call dsbtrd('N',uplo,n,ka,ab,ldab,d,e,x,ldx,work,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)
        End If
      End If

99999 Format (3X,(8F8.4))
    End Program f08uefe
```

10.2 Program Data

```
F08UEF Example Program Data
  4  2  1                        :Values of N, KA and KB
  'L'                            :Value of UPLO
  0.24
  0.39  -0.11
  0.42   0.79  -0.25
         0.63   0.48  -0.03      :End of matrix A
  2.07
  0.95   1.69
        -0.29   0.65
               -0.33   1.17      :End of matrix B
```

10.3 Program Results

```
 F08UEF Example Program Results

 Eigenvalues
    -0.8305 -0.6401  0.0992  1.8525
```