NAG C Library Function Document

nag_dspgst (f08tec)

1 Purpose

nag_dspgst (f08tec) reduces a real symmetric-definite generalized eigenproblem $Az = \lambda Bz$, $ABz = \lambda z$ or $BAz = \lambda z$ to the standard form $Cy = \lambda y$, where A is a real symmetric matrix and B has been factorized by nag_dpptrf (f07gdc), using packed storage.

2 Specification

```
#include <nag.h>
#include <nagf08.h>
```

```
void nag_dspgst (Nag_OrderType order, Nag_ComputeType comp_type,
     Nag_UploType uplo, Integer n, double ap[], const double bp[], NagError *fail)
```

3 Description

To reduce the real symmetric-definite generalized eigenproblem $Az = \lambda Bz$, $ABz = \lambda z$ or $BAz = \lambda z$ to the standard form $Cy = \lambda y$ using packed storage, this function must be preceded by a call to nag_dpptrf (f07gdc) which computes the Cholesky factorization of B; B must be positive-definite.

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

comp_type	Problem	**uplo**	B	C	z
1	$Az = \lambda Bz$	**Nag_Upper** **Nag_Lower**	$U^{\mathrm{T}}U$ LL^{T}	$U^{-\mathrm{T}}AU^{-1}$ $L^{-1}AL^{-\mathrm{T}}$	$U^{-1}y$ $L^{-\mathrm{T}}y$
2	$ABz = \lambda z$	**Nag_Upper** **Nag_Lower**	$U^{\mathrm{T}}U$ LL^{T}	UAU^{T} $L^{\mathrm{T}}AL$	$U^{-1}yL^{-\mathrm{T}}y$
3	$BAz = \lambda z$	**Nag_Upper** **Nag_Lower**	$U^{\mathrm{T}}U$ LL^{T}	UAU^{T} $L^{\mathrm{T}}AL$	$U^{\mathrm{T}}yLy$

4 References

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

5 Arguments

1: **order** – Nag_OrderType *Input*

On entry: the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = **Nag_RowMajor**. See Section 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this argument.

Constraint: **order** = **Nag_RowMajor** or **Nag_ColMajor**.

2: **comp_type** – Nag_ComputeType *Input*

On entry: indicates how the standard form is computed.

comp_type = **Nag_Compute_1**

if **uplo** = **Nag_Upper**, $C = U^{-\mathrm{T}} A U^{-1}$;
if **uplo** = **Nag_Lower**, $C = L^{-1} A L^{-\mathrm{T}}$.

comp_type = **Nag_Compute_2** or **Nag_Compute_3**

if **uplo** = **Nag_Upper**, $C = UAU^{\mathrm{T}}$;
if **uplo** = **Nag_Lower**, $C = L^{\mathrm{T}} A L$.

Constraint: **comp_type** = **Nag_Compute_1**, **Nag_Compute_2** or **Nag_Compute_3**.

3: **uplo** – Nag_UploType *Input*

On entry: indicates whether the upper or lower triangular part of A is stored and how B has been factorized.

uplo = **Nag_Upper**

The upper triangular part of A is stored and $B = U^{\mathrm{T}} U$.

uplo = **Nag_Lower**

The lower triangular part of A is stored and $B = LL^{\mathrm{T}}$.

Constraint: **uplo** = **Nag_Upper** or **Nag_Lower**.

4: **n** – Integer *Input*

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

Constraint: **n** ≥ 0.

5: **ap**[dim] – double *Input/Output*

Note: the dimension, *dim*, of the array **ap** must be at least $\max(1, \mathbf{n} \times (\mathbf{n} + 1)/2)$.

On entry: the symmetric matrix A, packed by rows or columns. The storage of elements a_{ij} depends on the **order** and **uplo** arguments as follows:

if **order** = **Nag_ColMajor** and **uplo** = **Nag_Upper**,
a_{ij} is stored in **ap**$[(j-1) \times j/2 + i - 1]$, for $i \leq j$;
if **order** = **Nag_ColMajor** and **uplo** = **Nag_Lower**,
a_{ij} is stored in **ap**$[(2n-j) \times (j-1)/2 + i - 1]$, for $i \geq j$;
if **order** = **Nag_RowMajor** and **uplo** = **Nag_Upper**,
a_{ij} is stored in **ap**$[(2n-i) \times (i-1)/2 + j - 1]$, for $i \leq j$;
if **order** = **Nag_RowMajor** and **uplo** = **Nag_Lower**,
a_{ij} is stored in **ap**$[(i-1) \times i/2 + j - 1]$, for $i \geq j$.

On exit: the upper or lower triangle of A is overwritten by the corresponding upper or lower triangle of C as specified by **comp_type** and **uplo**, using the same packed storage format as described above.

6: **bp**[dim] – const double *Input*

Note: the dimension, *dim*, of the array **bp** must be at least $\max(1, \mathbf{n} \times (\mathbf{n} + 1)/2)$.

On entry: the Cholesky factor of B as specified by **uplo** and returned by nag_dpptrf (f07gdc).

7: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 2.6 of the Essential Introduction).

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_INT

On entry, $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{n} \geq 0$.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

7 Accuracy

Forming the reduced matrix C is a stable procedure. However it involves implicit multiplication by B^{-1} if (**comp_type** = **Nag_Compute_1**) or B (if **comp_type** = **Nag_Compute_2** or **Nag_Compute_3**). When the function 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 Further Comments

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

The complex analogue of this function is nag_zhpgst (f08tsc).

9 Example

To compute all the eigenvalues of $Az = \lambda Bz$, where

$$A = \begin{pmatrix} 0.24 & 0.39 & 0.42 & -0.16 \\ 0.39 & -0.11 & 0.79 & 0.63 \\ 0.42 & 0.79 & -0.25 & 0.48 \\ -0.16 & 0.63 & 0.48 & -0.03 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.09 & 0.34 & 1.18 \end{pmatrix},$$

using packed storage. Here B is symmetric positive-definite and must first be factorized by nag_dpptrf (f07gdc). The program calls nag_dspgst (f08tec) to reduce the problem to the standard form $Cy = \lambda y$; then nag_dsptrd (f08gec) to reduce C to tridiagonal form, and nag_dsterf (f08jfc) to compute the eigenvalues.

9.1 Program Text

```
/* nag_dspgst (f08tec) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf07.h>
#include <nagf08.h>

int main(void)
{
  /* Scalars */
  Integer  i, j, n, ap_len, bp_len, d_len, e_len, tau_len;
  Integer  exit_status=0;
```

```
  NagError fail;
  Nag_UploType uplo;
  Nag_OrderType order;

  /* Arrays */
  char   uplo_char[2];
  double *ap=0, *bp=0, *d=0, *e=0, *tau=0;

#ifdef NAG_COLUMN_MAJOR
#define A_UPPER(I,J) ap[J*(J-1)/2 + I - 1]
#define A_LOWER(I,J) ap[(2*n-J)*(J-1)/2 + I - 1]
#define B_UPPER(I,J) bp[J*(J-1)/2 + I - 1]
#define B_LOWER(I,J) bp[(2*n-J)*(J-1)/2 + I - 1]
  order = Nag_ColMajor;
#else
#define A_LOWER(I,J) ap[I*(I-1)/2 + J - 1]
#define A_UPPER(I,J) ap[(2*n-I)*(I-1)/2 + J - 1]
#define B_LOWER(I,J) bp[I*(I-1)/2 + J - 1]
#define B_UPPER(I,J) bp[(2*n-I)*(I-1)/2 + J - 1]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);
  Vprintf("nag_dspgst (f08tec) Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
  ap_len = n * (n +1 )/2;
  bp_len = n * (n +1 )/2;
  d_len = n;
  e_len = n-1;
  tau_len = n;

  /* Allocate memory */
  if ( !(ap = NAG_ALLOC(ap_len, double)) ||
       !(bp = NAG_ALLOC(bp_len, double)) ||
       !(d = NAG_ALLOC(d_len, double)) ||
       !(e = NAG_ALLOC(e_len, double)) ||
       !(tau = NAG_ALLOC(tau_len, double)) )
    {
      Vprintf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Read A and B from data file */
  Vscanf(" ' %1s '%*[^\n] ", uplo_char);
  if (*(unsigned char *)uplo_char == 'L')
    uplo = Nag_Lower;
  else if (*(unsigned char *)uplo_char == 'U')
    uplo = Nag_Upper;
  else
    {
      Vprintf("Unrecognised character for Nag_UploType type\n");
      exit_status = -1;
      goto END;
    }
  if (uplo == Nag_Upper)
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            Vscanf("%lf", &A_UPPER(i,j));
        }
      Vscanf("%*[^\n] ");
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            Vscanf("%lf", &B_UPPER(i,j));
        }
```

```
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A_LOWER(i,j));
        }
      Vscanf("%*[^\n] ");
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &B_LOWER(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  /* Compute the Cholesky factorization of B */
  /* nag_dpptrf (f07gdc).
   * Cholesky factorization of real symmetric
   * positive-definite matrix, packed storage
   */
  nag_dpptrf(order, uplo, n, bp, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_dpptrf (f07gdc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Reduce the problem to standard form C*y = lambda*y, storing */
  /* the result in A */
  /* nag_dspgst (f08tec).
   * Reduction to standard form of real symmetric-definite
   * generalized eigenproblem Ax~=~lambda~Bx, ABx~=~lambda~x
   * or BAx~=~lambda~x, packed storage, B factorized by
   * nag_dpptrf (f07gdc)
   */
  nag_dspgst(order, Nag_Compute_1, uplo, n, ap, bp, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_dspgst (f08tec).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Reduce C to tridiagonal form T = (Q**T)*C*Q */
  /* nag_dsptrd (f08gec).
   * Orthogonal reduction of real symmetric matrix to
   * symmetric tridiagonal form, packed storage
   */
  nag_dsptrd(order, uplo, n, ap, d, e, tau, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_dsptrd (f08gec).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Calculate the eigenvalues of T (same as C) */
  /* nag_dsterf (f08jfc).
   * All eigenvalues of real symmetric tridiagonal matrix,
   * root-free variant of QL or QR
   */
  nag_dsterf(n, d, e, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_dsterf (f08jfc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print eigenvalues */
  Vprintf("Eigenvalues\n");
  for (i = 1; i <= n; ++i)
```

```
    Vprintf("%8.4f%s", d[i-1], i%9==0 || i==n ?"\n":" ");
  Vprintf("\n");
 END:
  if (ap) NAG_FREE(ap);
  if (bp) NAG_FREE(bp);
  if (d) NAG_FREE(d);
  if (e) NAG_FREE(e);
  if (tau) NAG_FREE(tau);

  return exit_status;
}
```

9.2 Program Data

```
nag_dspgst (f08tec) Example Program Data
  4                          :Value of N
  'L'                        :Value of UPLO
  0.24
  0.39  -0.11
  0.42   0.79  -0.25
 -0.16   0.63   0.48  -0.03   :End of matrix A
  4.16
 -3.12   5.03
  0.56  -0.83   0.76
 -0.10   1.09   0.34   1.18   :End of matrix B
```

9.3 Program Results

```
nag_dspgst (f08tec) Example Program Results

Eigenvalues
 -2.2254  -0.4548   0.1001   1.1270
```