NAG Library Function Document

nag_real_symm_sparse_eigensystem_monit (f12fec)

Note: *this function uses* **optional parameters** *to define choices in the problem specification. If you wish to use* default *settings for all of the optional parameters, then the option setting function nag_real_symm_sparse_eigensystem_option (f12fdc) need not be called. If, however, you wish to reset some or all of the settings please refer to Section 11 in nag_real_symm_sparse_eigensystem_option (f12fdc) for a detailed description of the specification of the optional parameters.*

1 Purpose

nag_real_symm_sparse_eigensystem_monit (f12fec) can be used to return additional monitoring information during computation. It is in a suite of functions which includes nag_real_symm_sparse_eigensystem_init (f12fac), nag_real_symm_sparse_eigensystem_iter (f12fbc), nag_real_symm_sparse_eigensystem_sol (f12fcc) and nag_real_symm_sparse_eigensystem_option (f12fdc).

2 Specification

```
#include <nag.h>
#include <nagf12.h>
void nag_real_symm_sparse_eigensystem_monit (Integer *niter, Integer *nconv,
     double ritz[], double rzest[], const Integer icomm[],
     const double comm[])
```

3 Description

The suite of functions is designed to calculate some of the eigenvalues, λ, (and optionally the corresponding eigenvectors, x) of a standard eigenvalue problem $Ax = \lambda x$, or of a generalized eigenvalue problem $Ax = \lambda Bx$ of order n, where n is large and the coefficient matrices A and B are sparse, real and symmetric. The suite can also be used to find selected eigenvalues/eigenvectors of smaller scale dense, real and symmetric problems.

On an intermediate exit from nag_real_symm_sparse_eigensystem_iter (f12fbc) with **irevcm** $= 4$, nag_real_symm_sparse_eigensystem_monit (f12fec) may be called to return monitoring information on the progress of the Arnoldi iterative process. The information returned by nag_real_symm_sparse_eigensystem_monit (f12fec) is:

– the number of the current Arnoldi iteration;

– the number of converged eigenvalues at this point;

– the real and imaginary parts of the converged eigenvalues;

– the error bounds on the converged eigenvalues.

nag_real_symm_sparse_eigensystem_monit (f12fec) does not have an equivalent function from the ARPACK package which prints various levels of detail of monitoring information through an output channel controlled via an argument value (see Lehoucq *et al.* (1998) for details of ARPACK routines). nag_real_symm_sparse_eigensystem_monit (f12fec) should not be called at any time other than immediately following an **irevcm** $= 4$ return from nag_real_symm_sparse_eigensystem_iter (f12fbc).

4 References

Lehoucq R B (2001) Implicitly restarted Arnoldi methods and subspace iteration *SIAM Journal on Matrix Analysis and Applications* **23** 551–562

Lehoucq R B and Scott J A (1996) An evaluation of software for computing eigenvalues of sparse nonsymmetric matrices *Preprint MCS-P547-1195* Argonne National Laboratory

Lehoucq R B and Sorensen D C (1996) Deflation techniques for an implicitly restarted Arnoldi iteration *SIAM Journal on Matrix Analysis and Applications* **17** 789–821

Lehoucq R B, Sorensen D C and Yang C (1998) *ARPACK Users' Guide: Solution of Large-scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods* SIAM, Philidelphia

5 Arguments

1: **niter** – Integer * *Output*

On exit: the number of the current Arnoldi iteration.

2: **nconv** – Integer * *Output*

On exit: the number of converged eigenvalues so far.

3: **ritz**[*dim*] – double *Output*

Note: the dimension, *dim*, of the array **ritz** must be at least **ncv** (see nag_real_symm_sparse_eigensystem_init (f12fac)).

On exit: the first **nconv** locations of the array **ritz** contain the real converged approximate eigenvalues.

4: **rzest**[*dim*] – double *Output*

Note: the dimension, *dim*, of the array **rzest** must be at least **ncv** (see nag_real_symm_sparse_eigensystem_init (f12fac)).

On exit: the first **nconv** locations of the array **rzest** contain the Ritz estimates (error bounds) on the real **nconv** converged approximate eigenvalues.

5: **icomm**[*dim*] – const Integer *Communication Array*

Note: the dimension, *dim*, of the array **icomm** must be at least max(1, **licomm**), where **licomm** is passed to the setup function (see nag_real_symm_sparse_eigensystem_init (f12fac)).

On entry: the array **icomm** output by the preceding call to nag_real_symm_sparse_eigensystem_iter (f12fbc).

6: **comm**[*dim*] – const double *Communication Array*

Note: the dimension, *dim*, of the array **comm** must be at least max(1, **lcomm**), where **lcomm** is passed to the setup function (see nag_real_symm_sparse_eigensystem_init (f12fac)).

On entry: the array **comm** output by the preceding call to nag_real_symm_sparse_eigensystem_iter (f12fbc).

6 Error Indicators and Warnings

None.

7 Accuracy

A Ritz value, λ, is deemed to have converged if its Ritz estimate $\leq$ **Tolerance** $\times |\lambda|$. The default **Tolerance** used is the ***machine precision*** given by nag_machine_precision (X02AJC).

8 Parallelism and Performance

nag_real_symm_sparse_eigensystem_monit (f12fec) is not threaded in any implementation.

9 Further Comments

None.

10 Example

This example solves $Kx = \lambda K_G x$ using the **Buckling** option (see nag_real_symm_sparse_eigensyste m_option (f12fdc), where K and K_G are obtained by the finite element method applied to the one-dimensional discrete Laplacian operator $\frac{\partial^2 u}{\partial x^2}$ on $[0, 1]$, with zero Dirichlet boundary conditions using piecewise linear elements. The shift, σ, is a real number, and the operator used in the Buckling iterative process is $\mathrm{OP} = \mathrm{inv}(K - \sigma K_G) \times K$ and $B = K$.

10.1 Program Text

```
/* nag_real_symm_sparse_eigensystem_monit (f12fec) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <stdio.h>
#include <nagf12.h>
#include <nagf16.h>

static void av(Integer, double *, double *);
static void my_dgttrf(Integer, double *, double *, double *,
                      double *, Integer *, Integer *);
static void my_dgttrs(Integer, double *, double *, double *,
                      double *, Integer *, double *, double *);

int main(void)
{
  /* Constants */
  Integer licomm = 140, imon = 1;

  /* Scalars */
  double estnrm, h, r1, r2, sigma;
  Integer exit_status, info, irevcm, j, lcomm, n, nconv, ncv;
  Integer nev, niter, nshift;
  /* Nag types */
  NagError fail;
  /* Arrays */
  double *dd = 0, *dl = 0, *du = 0, *du2 = 0, *comm = 0, *eigest = 0;
  double *eigv = 0, *resid = 0, *v = 0, *x2 = 0;
  Integer *icomm = 0, *ipiv = 0;
  /* Pointers */
  double *mx = 0, *x = 0, *y = 0;

  exit_status = 0;
  INIT_FAIL(fail);

  printf("nag_real_symm_sparse_eigensystem_monit (f12fec) Example "
         "Program Results\n");
  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

  /* Read values for nx, nev and cnv from data file. */
```

```
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &n, &nev, &ncv);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &n, &nev, &ncv);
#endif

  /* Allocate memory */
  lcomm = 3 * n + ncv * ncv + 8 * ncv + 60;
  if (!(dd = NAG_ALLOC(n, double)) ||
      !(dl = NAG_ALLOC(n, double)) ||
      !(du = NAG_ALLOC(n, double)) ||
      !(du2 = NAG_ALLOC(n, double)) ||
      !(comm = NAG_ALLOC(lcomm, double)) ||
      !(eigv = NAG_ALLOC(ncv, double)) ||
      !(eigest = NAG_ALLOC(ncv, double)) ||
      !(resid = NAG_ALLOC(n, double)) ||
      !(v = NAG_ALLOC(n * ncv, double)) ||
      !(x2 = NAG_ALLOC(n, double)) ||
      !(icomm = NAG_ALLOC(licomm, Integer)) ||
      !(ipiv = NAG_ALLOC(n, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Initialize communication arrays for problem using
     nag_real_symm_sparse_eigensystem_init (f12fac). */
  nag_real_symm_sparse_eigensystem_init(n, nev, ncv, icomm, licomm, comm,
                                        lcomm, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_real_symm_sparse_eigensystem_init "
           "(f12fac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
  /* Select the problem type using
     nag_real_symm_sparse_eigensystem_option (f12fdc). */
  nag_real_symm_sparse_eigensystem_option("generalized", icomm, comm, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_real_symm_sparse_eigensystem_option "
           "(f12fdc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Select the operating mode (Buckling) using
     nag_real_symm_sparse_eigensystem_option (f12fdc). */
  nag_real_symm_sparse_eigensystem_option("buckling", icomm, comm, &fail);

  /* Setup M and factorise */
  h = 1.0 / (double) (n + 1);
  r1 = 2.0 * h / 3.0;
  r2 = h / 6.0;
  sigma = 1.0;
  for (j = 0; j <= n - 1; ++j) {
    dd[j] = 2.0 / h - sigma * r1;
    dl[j] = -1.0 / h - sigma * r2;
    du[j] = dl[j];
  }
  my_dgttrf(n, dl, dd, du, du2, ipiv, &info);

  irevcm = 0;
REVCOMLOOP:
  /* Repeated calls to reverse communication routine
     nag_real_symm_sparse_eigensystem_iter (f12fbc). */
  nag_real_symm_sparse_eigensystem_iter(&irevcm, resid, v, &x, &y, &mx,
                                        &nshift, comm, icomm, &fail);
  if (irevcm != 5) {
    if (irevcm == -1) {
      /* Perform  y <--- OP*x = inv[K-SIGMA*KG]*K*x. */
```

```
      av(n, x, x2);
      my_dgttrs(n, dl, dd, du, du2, ipiv, x2, y);
    }
    else if (irevcm == 1) {
      /* Perform y <-- OP*x = inv[K-sigma*KG]*K*x. */
      my_dgttrs(n, dl, dd, du, du2, ipiv, mx, y);
    }
    else if (irevcm == 2) {
      /* Perform  y <--- K*x. */
      av(n, x, y);
    }
    else if (irevcm == 4 && imon == 1) {
      /* If imon=1, get monitoring information using
         nag_real_symm_sparse_eigensystem_monit (f12fec). */
      nag_real_symm_sparse_eigensystem_monit(&niter, &nconv, eigv, eigest,
                                              icomm, comm);
      /* Compute 2-norm of Ritz estimates using
         nag_dge_norm (f16rac). */
      nag_dge_norm(Nag_ColMajor, Nag_FrobeniusNorm, nev, 1, eigest, nev,
                   &estnrm, &fail);
      printf("Iteration %3" NAG_IFMT ", ", niter);
      printf(" No. converged = %3" NAG_IFMT ",", nconv);
      printf(" norm of estimates = %17.8e\n", estnrm);
    }
    goto REVCOMLOOP;
  }
  if (fail.code == NE_NOERROR) {
    /* Post-Process using nag_real_symm_sparse_eigensystem_sol
       (f12fcc) to compute eigenvalues/vectors. */
    nag_real_symm_sparse_eigensystem_sol(&nconv, eigv, v, sigma, resid, v,
                                          comm, icomm, &fail);
    printf("\n The %4" NAG_IFMT " generalized Ritz values", nconv);
    printf(" closest to %8.4f are:\n\n", sigma);
    for (j = 0; j <= nconv - 1; ++j) {
      printf("%8" NAG_IFMT "%5s%12.4f\n", j + 1, "", eigv[j]);
    }
  }
  else {
    printf(" Error from nag_real_symm_sparse_eigensystem_iter "
           "(f12fbc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
END:
  NAG_FREE(dd);
  NAG_FREE(dl);
  NAG_FREE(du);
  NAG_FREE(du2);
  NAG_FREE(comm);
  NAG_FREE(eigv);
  NAG_FREE(eigest);
  NAG_FREE(resid);
  NAG_FREE(v);
  NAG_FREE(x2);
  NAG_FREE(icomm);
  NAG_FREE(ipiv);

  return exit_status;
}

static void av(Integer n, double *v, double *y)
{
  /* Scalars */
  double h;
  Integer j;

  /* Function Body */
  h = (double) (n + 1);
  y[0] = h * (v[0] * 2.0 - v[1]);
  for (j = 1; j <= n - 2; ++j) {
    y[j] = h * (-v[j - 1] + v[j] * 2.0 - v[j + 1]);
```

```
  }
  y[n - 1] = h * (-v[n - 2] + v[n - 1] * 2.0);
  return;
} /* av */

static void my_dgttrf(Integer n, double dl[], double d[],
                      double du[], double du2[], Integer ipiv[],
                      Integer *info)
{
  /* A simple C version of the Lapack routine dgttrf with argument
     checking removed */
  /* Scalars */
  double temp, fact;
  Integer i;
  /* Function Body */
  *info = 0;
  for (i = 0; i < n; ++i) {
    ipiv[i] = i;
  }
  for (i = 0; i < n - 2; ++i) {
    du2[i] = 0.0;
  }
  for (i = 0; i < n - 2; i++) {
    if (fabs(d[i]) >= fabs(dl[i])) {
      /* No row interchange required, eliminate dl[i]. */
      if (d[i] != 0.0) {
        fact = dl[i] / d[i];
        dl[i] = fact;
        d[i + 1] = d[i + 1] - fact * du[i];
      }
    }
    else {
      /* Interchange rows I and I+1, eliminate dl[I] */
      fact = d[i] / dl[i];
      d[i] = dl[i];
      dl[i] = fact;
      temp = du[i];
      du[i] = d[i + 1];
      d[i + 1] = temp - fact * d[i + 1];
      du2[i] = du[i + 1];
      du[i + 1] = -fact * du[i + 1];
      ipiv[i] = i + 1;
    }
  }
  if (n > 1) {
    i = n - 2;
    if (fabs(d[i]) >= fabs(dl[i])) {
      if (d[i] != 0.0) {
        fact = dl[i] / d[i];
        dl[i] = fact;
        d[i + 1] = d[i + 1] - fact * du[i];
      }
    }
    else {
      fact = d[i] / dl[i];
      d[i] = dl[i];
      dl[i] = fact;
      temp = du[i];
      du[i] = d[i + 1];
      d[i + 1] = temp - fact * d[i + 1];
      ipiv[i] = i + 1;
    }
  }
  /* Check for a zero on the diagonal of U. */
  for (i = 0; i < n; ++i) {
    if (d[i] == 0.0) {
      *info = i;
      goto END;
    }
  }
END:
```

```
  return;
}

static void my_dgttrs(Integer n, double dl[], double d[],
                      double du[], double du2[], Integer ipiv[],
                      double b[], double y[])
{
  /* A simple C version of the Lapack routine dgttrs with argument
     checking removed, the number of right-hand-sides=1, Trans='N' */
  /* Scalars */
  Integer i, ip;
  double temp;
  /* Solve L*x = b. */
  for (i = 0; i <= n - 1; ++i) {
    y[i] = b[i];
  }
  for (i = 0; i < n - 1; ++i) {
    ip = ipiv[i];
    temp = y[i + 1 - ip + i] - dl[i] * y[ip];
    y[i] = y[ip];
    y[i + 1] = temp;
  }
  /* Solve U*x = b. */
  y[n - 1] = y[n - 1] / d[n - 1];
  if (n > 1) {
    y[n - 2] = (y[n - 2] - du[n - 2] * y[n - 1]) / d[n - 2];
  }
  for (i = n - 3; i >= 0; --i) {
    y[i] = (y[i] - du[i] * y[i + 1] - du2[i] * y[i + 2]) / d[i];
  }
  return;
}
```

10.2 Program Data

```
nag_real_symm_sparse_eigensystem_monit (f12fec) Example Program Data
 100  4  10 : Values for n, nev and ncv
```

10.3 Program Results

```
nag_real_symm_sparse_eigensystem_monit (f12fec) Example Program Results
Iteration   1,  No. converged =   0, norm of estimates =    2.05343313e-06
Iteration   2,  No. converged =   2, norm of estimates =    6.07599403e-11
Iteration   3,  No. converged =   3, norm of estimates =    5.26525802e-15

 The    4 generalized Ritz values closest to   1.0000 are:

       1          9.8704
       2         39.4912
       3         88.8909
       4        158.1175
```