NAG Library Function Document

nag_real_symm_sparse_eigensystem_init (f12fac)

1 Purpose

nag_real_symm_sparse_eigensystem_init (f12fac) is a setup function in a suite of functions consisting of nag_real_symm_sparse_eigensystem_init (f12fac), nag_real_symm_sparse_eigensystem_iter (f12fbc), nag_real_symm_sparse_eigensystem_sol (f12fcc), nag_real_symm_sparse_eigensystem_option (f12fdc) and nag_real_symm_sparse_eigensystem_monit (f12fec). It is used to find some of the eigenvalues (and optionally the corresponding eigenvectors) of a standard or generalized eigenvalue problem defined by real symmetric matrices.

The suite of functions is suitable for the solution of large sparse, standard or generalized, symmetric eigenproblems where only a few eigenvalues from a selected range of the spectrum are required.

2 Specification

```
#include <nag.h>
#include <nagf12.h>
void nag_real_symm_sparse_eigensystem_init (Integer n, Integer nev,
     Integer ncv, Integer icomm[], Integer licomm, double comm[],
     Integer lcomm, NagError *fail)
```

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.

nag_real_symm_sparse_eigensystem_init (f12fac) is a setup function which must be called before nag_real_symm_sparse_eigensystem_iter (f12fbc), the reverse communication iterative solver, and before nag_real_symm_sparse_eigensystem_option (f12fdc), the options setting function. nag_real_symm_sparse_eigensystem_sol (f12fcc), is a post-processing function that must be called following a successful final exit from nag_real_symm_sparse_eigensystem_iter (f12fbc), while nag_real_symm_sparse_eigensystem_monit (f12fec) can be used to return additional monitoring information during the computation.

This setup function initializes the communication arrays, sets (to their default values) all options that can be set by you via the option setting function nag_real_symm_sparse_eigensystem_option (f12fdc), and checks that the lengths of the communication arrays as passed by you are of sufficient length. For details of the options available and how to set them see Section 11.1 in nag_real_symm_sparse_eigensystem_option (f12fdc).

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: **n** – Integer *Input*

On entry: the order of the matrix A (and the order of the matrix B for the generalized problem) that defines the eigenvalue problem.

Constraint: $\mathbf{n} > 0$.

2: **nev** – Integer *Input*

On entry: the number of eigenvalues to be computed.

Constraint: $0 < \mathbf{nev} < \mathbf{n} - 1$.

3: **ncv** – Integer *Input*

On entry: the number of Lanczos basis vectors to use during the computation.

At present there is no *a priori* analysis to guide the selection of **ncv** relative to **nev**. However, it is recommended that $\mathbf{ncv} \geq 2 \times \mathbf{nev} + 1$. If many problems of the same type are to be solved, you should experiment with increasing **ncv** while keeping **nev** fixed for a given test problem. This will usually decrease the required number of matrix-vector operations but it also increases the work and storage required to maintain the orthogonal basis vectors. The optimal 'cross-over' with respect to CPU time is problem dependent and must be determined empirically.

Constraint: $\mathbf{nev} < \mathbf{ncv} \leq \mathbf{n}$.

4: **icomm**[**max**(**1**, **licomm**)] – Integer *Communication Array*

On exit: contains data to be communicated to the other functions in the suite.

5: **licomm** – Integer *Input*

On entry: the dimension of the array **icomm**.

If $\mathbf{licomm} = -1$, a workspace query is assumed and the function only calculates the required dimensions of **icomm** and **comm**, which it returns in **icomm**[0] and **comm**[0] respectively.

Constraint: $\mathbf{licomm} \geq 140$ or $\mathbf{licomm} = -1$.

6: **comm**[**max**(**1**, **lcomm**)] – double *Communication Array*

On exit: contains data to be communicated to the other functions in the suite.

7: **lcomm** – Integer *Input*

On entry: the dimension of the array **comm**.

If $\mathbf{lcomm} = -1$, a workspace query is assumed and the function only calculates the dimensions of **icomm** and **comm** required by nag_real_symm_sparse_eigensystem_iter (f12fbc), which it returns in **icomm**[0] and **comm**[0] respectively.

Constraint: $\mathbf{lcomm} \geq 3 \times \mathbf{n} + \mathbf{ncv} \times \mathbf{ncv} + 8 \times \mathbf{ncv} + 60$ or $\mathbf{lcomm} = -1$.

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

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.
See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** > 0.

On entry, **nev** = ⟨*value*⟩.
Constraint: **nev** > 0.

NE_INT_2

The length of the integer array **icomm** is too small **licomm** = ⟨*value*⟩, but must be at least ⟨*value*⟩.

NE_INT_3

On entry, **lcomm** = ⟨*value*⟩, **n** = ⟨*value*⟩ and **ncv** = ⟨*value*⟩.
Constraint: **lcomm** $\geq 3 \times$ **n** $+$ **ncv** $\times$ **ncv** $+ 8 \times$ **ncv** $+ 60$.

On entry, **ncv** = ⟨*value*⟩, **nev** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **ncv** $>$ **nev** and **ncv** $\leq$ **n**.

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 contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.
See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

Not applicable.

8 Parallelism and Performance

nag_real_symm_sparse_eigensystem_init (f12fac) is not threaded in any implementation.

9 Further Comments

None.

10 Example

This example solves $Ax = \lambda x$ in regular mode, where A is obtained from the standard central difference discretization of the Laplacian operator $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$ on the unit square, with zero Dirichlet boundary conditions. Eigenvalues of smallest magnitude are selected.

10.1 Program Text

```
/* nag_real_symm_sparse_eigensystem_init (f12fac) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

static void tv(Integer, double *, double *);
static void av(Integer, double *, double *);

int main(void)
{
  /* Constants */
  Integer imon = 0;
  /* Scalars */
  double sigma = 0, estnrm;
  Integer exit_status, irevcm, j, lcomm, licomm, n, nconv, ncv, nev;
  Integer niter, nshift, nx;
  /* Nag types */
  NagError fail;
  /* Arrays */
  double *comm = 0, *eigv = 0, *eigest = 0;
  double *resid = 0, *v = 0;
  Integer *icomm = 0;
  /* Ponters */
  double *mx = 0, *x = 0, *y = 0;

  exit_status = 0;
  INIT_FAIL(fail);

  printf("nag_real_symm_sparse_eigensystem_init (f12fac) 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] ", &nx, &nev, &ncv);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &nx, &nev, &ncv);
#endif

  /* Allocate memory */
  n = nx * nx;
  if (!(eigv = NAG_ALLOC(ncv, double)) ||
      !(eigest = NAG_ALLOC(ncv, double)) ||
      !(resid = NAG_ALLOC(n, double)) || !(v = NAG_ALLOC(n * ncv, double)))
  {
```

```
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }
  /* Initialize communication arrays for problem using
     nag_real_symm_sparse_eigensystem_init (f12fac).
     The first call sets lcomm = licomm = -1 to perform a workspace
     query. */
  lcomm = licomm = -1;
  if (!(comm = NAG_ALLOC(1, double)) || !(icomm = NAG_ALLOC(1, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }
  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;
  }
  lcomm = (Integer) comm[0];
  licomm = icomm[0];
  NAG_FREE(comm);
  NAG_FREE(icomm);
  if (!(comm = NAG_ALLOC(lcomm, double)) ||
      !(icomm = NAG_ALLOC(licomm, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }
  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 required spectrum using
     nag_real_symm_sparse_eigensystem_option (f12fdc). */
  nag_real_symm_sparse_eigensystem_option("smallest magnitude", 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;
  }
  /* Increase the iteration limit if required. */
  nag_real_symm_sparse_eigensystem_option("iteration limit=500", 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;
  }
  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 (fail.code != NE_NOERROR) {
    printf("Error from nag_real_symm_sparse_eigensystem_iter "
```

```
            "(f12fbc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
  if (irevcm != 5) {
    if (irevcm == -1 || irevcm == 1) {
      /* Perform matrix vector multiplication y <--- Op*x */
      av(nx, 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);
      if (fail.code != NE_NOERROR) {
        printf("Error from nag_dge_norm (f16rac).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
      }
      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);
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_real_symm_sparse_eigensystem_sol "
             "(f12fcc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
    printf("\n\n The %4" NAG_IFMT " Ritz values", nconv);
    printf(" of smallest magnitude are:\n\n");
    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(comm);
  NAG_FREE(eigv);
  NAG_FREE(eigest);
  NAG_FREE(resid);
  NAG_FREE(v);
  NAG_FREE(icomm);

  return exit_status;
}

static void av(Integer nx, double *v, double *w)
{
  /* Scalars */
  double nx2;
  Integer j, lo;
  /* Nag types */
  NagError fail;
  /* Function Body */
```

```
  INIT_FAIL(fail);
  nx2 = ((double) ((nx + 1) * (nx + 1)));
  tv(nx, v, w);
  nag_daxpby(nx, -nx2, &v[nx], 1, nx2, w, 1, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_daxpby (f16ecc).\n%s\n", fail.message);
    goto END;
  }
  for (j = 1; j <= nx - 2; ++j) {
    lo = j * nx;
    tv(nx, &v[lo], &w[lo]);
    nag_daxpby(nx, -nx2, &v[lo - nx], 1, nx2, &w[lo], 1, &fail);
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_daxpby (f16ecc).\n%s\n", fail.message);
      goto END;
    }
    nag_daxpby(nx, -nx2, &v[lo + nx], 1, 1.0, &w[lo], 1, &fail);
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_daxpby (f16ecc).\n%s\n", fail.message);
      goto END;
    }
  }
  lo = (nx - 1) * nx;
  tv(nx, &v[lo], &w[lo]);
  nag_daxpby(nx, -nx2, &v[lo - nx], 1, nx2, &w[lo], 1, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_daxpby (f16ecc).\n%s\n", fail.message);
    goto END;
  }
END:
  return;
} /* av */

static void tv(Integer nx, double *x, double *y)
{
  /* Compute the matrix vector multiplication y<---T*x where T is a nx */
  /* by nx tridiagonal matrix with constant diagonals (dd, dl and du). */
  /* Scalars */
  double dd, dl, du;
  Integer j;
  /* Function Body */
  dd = 4.0;
  dl = -1.0;
  du = -1.0;
  y[0] = dd * x[0] + du * x[1];
  for (j = 1; j <= nx - 2; ++j) {
    y[j] = dl * x[j - 1] + dd * x[j] + du * x[j + 1];
  }
  y[nx - 1] = dl * x[nx - 2] + dd * x[nx - 1];
  return;
} /* tv */
```

10.2 Program Data

```
nag_real_symm_sparse_eigensystem_init (f12fac) Example Program Data
 10  4  10 : Values for nx, nev and ncv
```

10.3 Program Results

```
nag_real_symm_sparse_eigensystem_init (f12fac) Example Program Results


 The    4 Ritz values of smallest magnitude are:

       1          19.6054
       2          48.2193
       3          48.2193
       4          76.8333
```