

NAG Library Routine Document

F12FAF

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

F12FAF is a setup routine in a suite of routines consisting of F12FAF, F12FBB, F12FCF, F12FDF and F12FEF. 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 routines 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

```
SUBROUTINE F12FAF (N, NEV, NCV, ICOMM, LICOMM, COMM, LCOMM, IFAIL)
INTEGER          N, NEV, NCV, ICOMM(max(1,LICOMM)), LICOMM, LCOMM, IFAIL
REAL (KIND=nag_wp) COMM(max(1,LCOMM))
```

3 Description

The suite of routines 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.

F12FAF is a setup routine which must be called before F12FBB, the reverse communication iterative solver, and before F12FDF, the options setting routine. F12FCF, is a post-processing routine that must be called following a successful final exit from F12FBB, while F12FEF can be used to return additional monitoring information during the computation.

This setup routine initializes the communication arrays, sets (to their default values) all options that can be set by you via the option setting routine F12FDF, 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 10.1 in F12FDF.

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, Philadelphia

5 Parameters

- 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: $N > 0$.
- 2: NEV – INTEGER *Input*
On entry: the number of eigenvalues to be computed.
Constraint: $0 < NEV < N - 1$.
- 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 $NCV \geq 2 \times NEV + 1$. 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: $NEV < NCV \leq N$.
- 4: ICOMM(max(1, LICOMM)) – INTEGER array *Communication Array*
On exit: contains data to be communicated to the other routines in the suite.
- 5: LICOMM – INTEGER *Input*
On entry: the dimension of the array ICOMM as declared in the (sub)program from which F12FAF is called.
 If LICOMM = -1, a workspace query is assumed and the routine only calculates the required dimensions of ICOMM and COMM, which it returns in ICOMM(1) and COMM(1) respectively.
Constraint: LICOMM ≥ 140 or LICOMM = -1.
- 6: COMM(max(1, LCOMM)) – REAL (KIND=nag_wp) array *Communication Array*
On exit: contains data to be communicated to the other routines in the suite.
- 7: LCOMM – INTEGER *Input*
On entry: the dimension of the array COMM as declared in the (sub)program from which F12FAF is called.
 If LCOMM = -1, a workspace query is assumed and the routine only calculates the dimensions of ICOMM and COMM required by F12FBF, which it returns in ICOMM(1) and COMM(1) respectively.
Constraint: LCOMM $\geq 3 \times N + NCV \times NCV + 8 \times NCV + 60$ or LCOMM = -1.
- 8: IFAIL – INTEGER *Input/Output*
On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.
 For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, $N \leq 0$.

IFAIL = 2

On entry, $NEV \leq 0$.

IFAIL = 3

On entry, $NCV \leq NEV$ or $NCV > N$.

IFAIL = 4

On entry, $LICOMM < 140$ and $LICOMM \neq -1$.

IFAIL = 5

On entry, $LCOMM < 3 \times N + NCV \times NCV + 8 \times NCV + 60$ and $LCOMM \neq -1$.

7 Accuracy

Not applicable.

8 Further Comments

None.

9 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.

9.1 Program Text

```
! F12FAF Example Program Text
! Mark 24 Release. NAG Copyright 2012.

Module f12faf_mod

! F12FAF Example Program Module:
! Parameters and User-defined Routines

! .. Use Statements ..
Use nag_library, Only: nag_wp
! .. Implicit None Statement ..
Implicit None
! .. Parameters ..
Real (Kind=nag_wp), Parameter :: one = 1.0_nag_wp
Integer, Parameter :: imon = 0, ipoint = 0, &
licomm = 140, nin = 5, nout = 6

Contains
```

```

Subroutine tv(nx,x,y)
!   Compute the matrix vector multiplication  $y \leftarrow -T*x$  where T is a nx
!   by nx tridiagonal matrix.

!   .. Scalar Arguments ..
Integer, Intent (In)           :: nx
!   .. Array Arguments ..
Real (Kind=nag_wp), Intent (In)  :: x(nx)
Real (Kind=nag_wp), Intent (Out) :: y(nx)
!   .. Local Scalars ..
Real (Kind=nag_wp)             :: dd, dl, du
Integer                         :: j
!   .. Executable Statements ..
dd = 4.0_nag_wp
dl = -one
du = -one
y(1) = dd*x(1) + du*x(2)
Do j = 2, nx - 1
  y(j) = dl*x(j-1) + dd*x(j) + du*x(j+1)
End Do
y(nx) = dl*x(nx-1) + dd*x(nx)
Return
End Subroutine tv
Subroutine av(nx,v,w)

!   .. Use Statements ..
Use nag_library, Only: daxpy, dscal
!   .. Scalar Arguments ..
Integer, Intent (In)           :: nx
!   .. Array Arguments ..
Real (Kind=nag_wp), Intent (In)  :: v(nx*nx)
Real (Kind=nag_wp), Intent (Out) :: w(nx*nx)
!   .. Local Scalars ..
Real (Kind=nag_wp)             :: h2
Integer                         :: j, lo, n
!   .. Intrinsic Procedures ..
Intrinsic                       :: real
!   .. Executable Statements ..
h2 = one/real((nx+1)*(nx+1),kind=nag_wp)
Call tv(nx,v(1),w(1))
!   The NAG name equivalent of daxpy is f06ecf
Call daxpy(nx,-one,v(nx+1),1,w(1),1)
Do j = 2, nx - 1
  lo = (j-1)*nx
  Call tv(nx,v(lo+1),w(lo+1))
  Call daxpy(nx,-one,v(lo-nx+1),1,w(lo+1),1)
  Call daxpy(nx,-one,v(lo+nx+1),1,w(lo+1),1)
End Do
lo = (nx-1)*nx
Call tv(nx,v(lo+1),w(lo+1))
Call daxpy(nx,-one,v(lo-nx+1),1,w(lo+1),1)
n = nx*nx
!   The NAG name equivalent of dscal is f06edf
Call dscal(n,one/h2,w,1)
Return
End Subroutine av
End Module f12fafa_mod
Program f12fafa

!   F12FAF Example Main Program

!   .. Use Statements ..
Use nag_library, Only: dnrn2, f12faf, f12fbf, f12fcf, f12fdf, f12fef, &
  nag_wp
Use f12fafa_mod, Only: av, imon, ipoint, licomm, nin, nout
!   .. Implicit None Statement ..
Implicit None
!   .. Local Scalars ..
Real (Kind=nag_wp)             :: sigma
Integer                         :: ifail, irevcm, j, lcomm, ldv, n, &
  nconv, ncv, nev, niter, nshift, nx

```

```

! .. Local Arrays ..
Real (Kind=nag_wp), Allocatable      :: ax(:), comm(:), d(:,,:), mx(:), &
                                     resid(:), v(:,,:), x(:)
Integer                               :: icomm(licomm)
! .. Executable Statements ..
Write (nout,*) 'F12FAF Example Program Results'
Write (nout,*)
! Skip heading in data file
Read (nin,*)
Read (nin,*) nx, nev, ncv

n = nx*nx
ldv = n
lcomm = 3*n + ncv*ncv + 8*ncv + 60
Allocate (ax(n),comm(lcomm),d(ncv,2),mx(n),resid(n),v(ldv,ncv),x(n))

ifail = 0
Call f12faf(n,nev,ncv,icomm,licomm,comm,lcomm,ifail)

ifail = 0
Call f12fdf('SMALLEST MAGNITUDE',icomm,comm,ifail)
! Increase the iteration limit if required.
Call f12fdf('ITERATION LIMIT=500',icomm,comm,ifail)
If (ipoint==1) Then
! Use pointers to Workspace in calculating matrix vector
! products rather than interfacing through the array X.
Call f12fdf('POINTERS=YES',icomm,comm,ifail)
End If

irevcm = 0
ifail = -1
revcm: Do
Call f12fbf(irevcm,resid,v,ldv,x,mx,nshift,comm,icomm,ifail)
If (irevcm==5) Then
Exit revcm
Else If (irevcm==-1 .Or. irevcm==1) Then
! Perform matrix vector multiplication y <--- Op*x
If (ipoint==0) Then
Call av(nx,x,ax)
x(1:n) = ax(1:n)
Else
Call av(nx,comm(icomm(1)),comm(icomm(2)))
End If
Else If (irevcm==4 .And. imon/=0) Then
! Output monitoring information
Call f12fef(niter,nconv,d,d(1,2),icomm,comm)
! The NAG name equivalent of dnrms is f06ejf
Write (6,99999) niter, nconv, dnrms(nev,d(1,2),1)
End If
End Do revcm

If (ifail==0) Then
! Post-Process using F12FCF to compute eigenvalue/vectors.
ifail = 0
Call f12fcf(nconv,d,v,ldv,sigma,resid,v,ldv,comm,icomm,ifail)
Write (nout,99998) nconv
Write (nout,99997)(j,d(j,1),j=1,nconv)
End If

99999 Format (1X,'Iteration',1X,I3,', No. converged =',1X,I3,', norm o', &
'f estimates =',E16.8)
99998 Format (1X/' The ',I4,' Ritz values of smallest magnitude are: '/')
99997 Format (1X,I8,5X,F12.4)
End Program f12fafa

```

9.2 Program Data

F12FAF Example Program Data
10 4 10 : Values for NX NEV and NCV

9.3 Program Results

F12FAF Example Program Results

The 4 Ritz values of smallest magnitude are:

1	19.6054
2	48.2193
3	48.2193
4	76.8333
