

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, F12FBF, 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,
1 IFAIL
  double precision 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 F12FBF, 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 F12FBF, 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 10.2 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 varying 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)) – **double precision** 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.
On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

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.**

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 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          IMON, IPOINT, LICOMM, NIN, NOUT
      PARAMETER        (IMON=0, IPOINT=0, LICOMM=140, NIN=5, NOUT=6)
      INTEGER          MAXN, MAXNCV, LDV
      PARAMETER        (MAXN=256, MAXNCV=30, LDV=MAXN)
      INTEGER          LCOMM
      PARAMETER        (LCOMM=3*MAXN+MAXNCV*MAXNCV+8*MAXNCV+60)
*      .. Local Scalars ..
      DOUBLE PRECISION SIGMA
      INTEGER          IFAIL, IREVCM, J, N, NCONV, NCV, NEV, NITER,
+                     NSHIFT, NX
*      .. Local Arrays ..
      DOUBLE PRECISION AX(MAXN), COMM(LCOMM), D(MAXNCV,2), MX(MAXN),
+                     RESID(MAXN), V(LDV,MAXNCV), X(MAXN)
      INTEGER          ICOMM(LICOMM)
```

```

*      .. External Functions ..
      DOUBLE PRECISION DNRM2
      EXTERNAL          DNRM2
*      .. External Subroutines ..
      EXTERNAL          AV, DCOPY, F12FAF, F12FBF, F12FCF, F12FDF, F12FEF
*      .. 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
      IF (N.LT.1 .OR. N.GT.MAXN) THEN
        WRITE (NOUT,99999) 'N is out of range: N = ', N
      ELSE IF (NCV.GT.MAXNCV) THEN
        WRITE (NOUT,99999) 'NCV is out of range: NCV = ', NCV
      ELSE
        IFAIL = 1
        CALL F12FAF(N,NEV,NCV,ICOMM,LICOMM,COMM,LCOMM,IFAIL)
*
*      IF (IFAIL.EQ.0) THEN
*      Set the region of the spectrum that is required.
        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.EQ.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
20      CONTINUE
        CALL F12FBF(IREVCM,RESID,V,LDV,X,MX,NSHIFT,COMM,ICOMM,IFAIL)
        IF (IREVCM.NE.5) THEN
          IF (IREVCM.EQ.-1 .OR. IREVCM.EQ.1) THEN
*      Perform matrix vector multiplication y <--- Op*x
          IF (IPOINT.EQ.0) THEN
            CALL AV(NX,X,AX)
            CALL DCOPY(N,AX,1,X,1)
          ELSE
            CALL AV(NX,COMM(ICOMM(1)),COMM(ICOMM(2)))
          END IF
          ELSE IF (IREVCM.EQ.4 .AND. IMON.NE.0) THEN
*      Output monitoring information
            CALL F12FEF(NITER,NCONV,D,D(1,2),ICOMM,COMM)
            WRITE (6,99998) NITER, NCONV, DNRM2(NEV,D(1,2),1)
          END IF
          GO TO 20
        END IF
        IF (IFAIL.EQ.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,99996) NCONV
          DO 40 J = 1, NCONV
            WRITE (NOUT,99995) J, D(J,1)
40          CONTINUE
        END IF
      ELSE
        WRITE (NOUT,99997) IFAIL
      END IF
    END IF
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,'Iteration',1X,I3,',', No. converged =',1X,I3,',', norm o',
+      'f estimates =',E16.8)
99997 FORMAT (1X,' ** F12FAF returned with IFAIL = ',I5)
99996 FORMAT (1X,/' The ',I4,' Ritz values of smallest magnitude are:',

```

```

+      /)
99995 FORMAT (1X,I8,5X,F12.4)
END

*
SUBROUTINE AV(NX,V,W)
*
.. Parameters ..
DOUBLE PRECISION ONE
PARAMETER      (ONE=1.0D+0)
*
.. Scalar Arguments ..
INTEGER        NX
*
.. Array Arguments ..
DOUBLE PRECISION V(NX*NX), W(NX*NX)
*
.. Local Scalars ..
DOUBLE PRECISION H2
INTEGER          J, LO
*
.. External Subroutines ..
EXTERNAL        DAXPY, DSCAL, TV
*
.. Intrinsic Functions ..
INTRINSIC       DBLE
*
.. Executable Statements ..
H2 = ONE/DBLE((NX+1)*(NX+1))
CALL TV(NX,V(1),W(1))
CALL DAXPY(NX,-ONE,V(NX+1),1,W(1),1)
DO 20 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)
20 CONTINUE
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)
CALL DSCAL(NX*NX,ONE/H2,W,1)
RETURN
END

*
SUBROUTINE TV(NX,X,Y)
*
Compute the matrix vector multiplication  $y \leftarrow T \cdot x$  where T is a nx
*
by nx tridiagonal matrix.
*
.. Parameters ..
DOUBLE PRECISION ONE
PARAMETER      (ONE=1.0D+0)
*
.. Scalar Arguments ..
INTEGER        NX
*
.. Array Arguments ..
DOUBLE PRECISION X(NX), Y(NX)
*
.. Local Scalars ..
DOUBLE PRECISION DD, DL, DU
INTEGER          J
*
.. Executable Statements ..
DD = 4.0D+0
DL = -ONE
DU = -ONE
Y(1) = DD*X(1) + DU*X(2)
DO 20 J = 2, NX - 1
    Y(J) = DL*X(J-1) + DD*X(J) + DU*X(J+1)
20 CONTINUE
Y(NX) = DL*X(NX-1) + DD*X(NX)
RETURN
END

```

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
