

NAG Toolbox for MATLAB

f12ap

1 Purpose

f12ap is an iterative solver in a suite of functions consisting of f12an, f12ap, f12aq, f12ar and f12as. It is used to find some of the eigenvalues (and optionally the corresponding eigenvectors) of a standard or generalized eigenvalue problem defined by complex nonsymmetric matrices.

2 Syntax

```
[irevcm, resid, v, x, mx, nshift, comm, icomm, ifail] = f12ap(irevcm,
resid, v, x, mx, comm, icomm)
```

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, complex and nonsymmetric. The suite can also be used to find selected eigenvalues/eigenvectors of smaller scale dense, complex and nonsymmetric problems.

f12ap is a **reverse communication** function, based on the ARPACK routine **znaupd**, using the Implicitly Restarted Arnoldi iteration method. The method is described in Lehoucq and Sorensen 1996 and Lehoucq 2001 while its use within the ARPACK software is described in great detail in Lehoucq *et al.* 1998. An evaluation of software for computing eigenvalues of sparse nonsymmetric matrices is provided in Lehoucq and Scott 1996. This suite of functions offers the same functionality as the ARPACK software for complex nonsymmetric problems, but the interface design is quite different in order to make the option setting clearer to you and to simplify the interface of f12ap.

The setup function f12an must be called before f12ap, the reverse communication iterative solver. Options may be set for f12ap by prior calls to the option setting function f12ar and a post-processing function f12aq must be called following a successful final exit from f12ap. f12as may be called following certain flagged intermediate exits from f12ap to provide additional monitoring information about the computation.

f12ap uses **reverse communication**, i.e., it returns repeatedly to the calling program with the parameter **irevcm** (see Section 5) set to specified values which require the calling program to carry out one of the following tasks:

- compute the matrix-vector product $y = OPx$, where OP is defined by the computational mode;
- compute the matrix-vector product $y = Bx$;
- notify the completion of the computation;
- allow the calling program to monitor the solution.

The problem type to be solved (standard or generalized), the spectrum of eigenvalues of interest, the mode used (regular, regular inverse, shifted inverse, shifted real or shifted imaginary) and other options can all be set using the option setting function f12ar (see Section 10.2 of the document for f12ar for details on setting options and of the default settings).

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

Note: this function uses **reverse communication**. Its use involves an initial entry, intermediate exits and re-entries, and a final exit, as indicated by the **parameter IREVCN**. Between intermediate exits and re-entries, **all parameters other than x, mx and comm must remain unchanged**.

5.1 Compulsory Input Parameters

1: **irevcn** – **int32 scalar**

On initial entry: **irevcn** = 0, otherwise an error condition will be raised.

On intermediate re-entry: must be unchanged from its previous exit value. Changing **irevcn** to any other value between calls will result in an error.

Constraint: on initial entry, **irevcn** = 0; on re-entry **irevcn** must remain unchanged.

2: **resid(*)** – **complex array**

Note: the dimension of the array **resid** must be at least **n** (see f12an).

On initial entry: need not be set unless the option **Initial Residual** has been set in a prior call to f12ar in which case **resid** should contain an initial residual vector, possibly from a previous run.

On intermediate re-entry: must be unchanged from its previous exit. Changing **resid** to any other value between calls may result in an error exit.

3: **v(ldv,*)** – **complex array**

The first dimension of the array **v** must be at least **n**

The second dimension of the array must be at least $\max(1, \mathbf{ncv})$

On initial entry: need not be set.

On intermediate re-entry: must be unchanged from its previous exit.

4: **x(*)** – **complex array**

Note: the dimension of the array **x** must be at least **n** (see f12an).

On initial entry: need not be set, it is used as a convenient mechanism for accessing elements of **comm**.

On intermediate re-entry: if **Pointers** = Yes, **x** need not be set.

If **Pointers** = No, **x** must contain the result of $y = OPx$ when **irevcn** returns the value -1 or $+1$. It must return the computed shifts when **irevcn** returns the value 3.

5: **mx(*)** – **complex array**

Note: the dimension of the array **mx** must be at least **n** (see f12an).

On initial entry: need not be set, it is used as a convenient mechanism for accessing elements of **comm**.

On intermediate re-entry: if **Pointers** = Yes, **mx** need not be set.

If **Pointers** = No, **mx** must contain the result of $y = Bx$ when **irevcn** returns the value 2.

6: **comm(*) – complex array**

Note: the dimension of the array **comm** must be at least $\max(1, 3 \times \mathbf{n} + 3 \times \mathbf{ncv} \times \mathbf{ncv} + 5 \times \mathbf{ncv} + 60)$ (see f12an).

On initial entry: must remain unchanged following a call to the setup function f12an.

7: **icomm(*) – int32 array**

Note: the dimension of the array **icomm** must be at least $\max(1, \mathbf{licomm})$ (see f12an).

On initial entry: must remain unchanged following a call to the setup function f12an.

5.2 Optional Input Parameters

None.

5.3 Input Parameters Omitted from the MATLAB Interface

ldv

5.4 Output Parameters1: **irevcn – int32 scalar**

On intermediate exit: has the following meanings.

- 1 The calling program must compute the matrix-vector product $y = OPx$, where x is stored in **x** (by default) or in the array **comm** (starting from the location given by the first element of **icomm**) when the option **Pointers** = Yes is set in a prior call to f12ar. The result y is returned in **x** (by default) or in the array **comm** (starting from the location given by the second element of **icomm**) when the option **Pointers** = Yes is set.
- 1 The calling program must compute the matrix-vector product $y = OPx$. This is similar to the case **irevcn** = –1 except that the result of the matrix-vector product $y = Bx$ (as required in some computational modes) has already been computed and is available in **mx** (by default) or in the array **comm** (starting from the location given by the third element of **icomm**) when the option **Pointers** = Yes is set.
- 2 The calling program must compute the matrix-vector product $y = Bx$, where x is stored in **x** and y is returned in **mx** (by default) or in the array **comm** (starting from the location given by the second element of **icomm**) when the option **Pointers** = Yes is set.
- 3 Compute the **nshift** complex shifts. This value of **irevcn** will only arise if the optional parameter **Supplied Shifts** is set in a prior call to f12ar which is intended for experienced users only; the default and recommended option is to use exact shifts (see Lehoucq *et al.* 1998 for details).
- 4 Monitoring step: a call to f12as can now be made to return the number of Arnoldi iterations, the number of converged Ritz values, the array of converged values, and the corresponding Ritz estimates.

On final exit: **irevcn** = 5: f12ap has completed its tasks. The value of **ifail** determines whether the iteration has been successfully completed, or whether errors have been detected. On successful completion f12aq must be called to return the requested eigenvalues and eigenvectors (and/or Schur vectors).

2: **resid(*) – complex array**

Note: the dimension of the array **resid** must be at least **n** (see f12an).

On intermediate exit: contains the current residual vector.

On final exit: contains the final residual vector.

3: **v(ldv,*) – complex array**

The first dimension of the array **v** must be at least **n**

The second dimension of the array must be at least $\max(1, \mathbf{ncv})$

On intermediate exit: contains the current set of Arnoldi basis vectors.

On final exit: contains the final set of Arnoldi basis vectors.

4: **x(*) – complex array**

Note: the dimension of the array **x** must be at least **n** (see f12an).

On intermediate exit: if **Pointers** = Yes, **x** is not referenced.

If **Pointers** = No, **x** contains the vector x when **irevcn** returns the value -1 or $+1$.

On final exit: does not contain useful data.

5: **mx(*) – complex array**

Note: the dimension of the array **mx** must be at least **n** (see f12an).

On intermediate exit: if **Pointers** = Yes, **mx** is not referenced.

If **Pointers** = No, **mx** contains the vector Bx when **irevcn** returns the value $+1$.

On final exit: does not contain any useful data.

6: **nshift – int32 scalar**

On intermediate exit: if the option **Supplied Shifts** is set and **irevcn** returns a value of 3, **nshift** returns the number of complex shifts required.

7: **comm(*) – complex array**

Note: the dimension of the array **comm** must be at least $\max(1, 3 \times \mathbf{n} + 3 \times \mathbf{ncv} \times \mathbf{ncv} + 5 \times \mathbf{ncv} + 60)$ (see f12an).

Contains data defining the current state of the iterative process.

8: **icomm(*) – int32 array**

Note: the dimension of the array **icomm** must be at least $\max(1, \mathbf{licomm})$ (see f12an).

Contains data defining the current state of the iterative process.

9: **ifail – int32 scalar**

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail = 1

On initial entry, the maximum number of iterations ≤ 0 , the option **Iteration Limit** has been set to a nonpositive value.

ifail = 2

The options **Generalized** and **Regular** are incompatible.

ifail = 3

The option **Initial Residual** was selected but the starting vector held in **resid** is zero.

ifail = 4

The maximum number of iterations has been reached. Some Ritz values may have converged; a subsequent call to f12aq will return the number of converged values and the converged values.

ifail = 5

No shifts could be applied during a cycle of the implicitly restarted Arnoldi iteration. One possibility is to increase the size of **nev** relative to **ncv** (see Section 5 of the document for f12an for details of these parameters).

ifail = 6

Could not build a Arnoldi factorization. Consider changing **nev** or **ncv** in the initialization function (see Section 5 of the document for f12an for details of these parameters).

ifail = 7

Unexpected error in internal call to compute eigenvalues and corresponding error bounds of the current upper Hessenberg matrix. Please contact NAG.

ifail = 8

Either the initialization function f12an has not been called prior to the first call of this function or a communication array has become corrupted.

ifail = 9

An unexpected error has occurred. Please contact NAG.

7 Accuracy

The relative accuracy of a Ritz value, λ , is considered acceptable if its Ritz estimate $\leq \textbf{Tolerance} \times |\lambda|$. The default **Tolerance** used is the *machine precision* given by x02aj.

8 Further Comments

None.

9 Example

```
n = int32(100);
nx = int32(10);
nev = int32(4);
ncv = int32(20);

irevcm = int32(0);
resid = complex(zeros(100,1));
v = complex(zeros(100,20));
x = complex(zeros(100,1));
mx = complex(zeros(100,1));

sigma = complex(0);

% Initialisation Step
[icomm, comm, ifail] = f12an(n, nev, ncv);

% Solve
while (irevcm ~= 5)
    [irevcm, resid, v, x, mx, nshift, comm, icomm, ifail] = ...
        f12ap(irevcm, resid, v, x, mx, comm, icomm);
```

```

    if (irevcm == 1 || irevcm == -1)
        x = f12_av(nx, x);
    elseif (irevcm == 4)
        [niter, nconv, ritz, rzest] = f12as(icom, comm);
        fprintf('Iteration %d, No. converged = %d, norm of estimates = %16.8g\n', niter, nconv, norm(rzest(1:nev),2));
    end
end

% Post-process to compute eigenvalues/vectors
[nconv, d, z, v, comm, ifail] = f12aq(sigma, resid, v, comm, icom);
% sort to avoid difference in order showing as an error

Iteration 1, No. converged = 0, norm of estimates = 132.04155
Iteration 2, No. converged = 0, norm of estimates = 102.2167
Iteration 3, No. converged = 0, norm of estimates = 61.46018
Iteration 4, No. converged = 0, norm of estimates = 23.673492
Iteration 5, No. converged = 0, norm of estimates = 6.7565006
Iteration 6, No. converged = 0, norm of estimates = 1.8830144
Iteration 7, No. converged = 0, norm of estimates = 0.48683436
Iteration 8, No. converged = 0, norm of estimates = 0.11166714
Iteration 9, No. converged = 0, norm of estimates = 0.033214754
Iteration 10, No. converged = 0, norm of estimates = 0.0086903151
Iteration 11, No. converged = 0, norm of estimates = 0.0015400799
Iteration 12, No. converged = 0, norm of estimates = 0.00041464548
Iteration 13, No. converged = 0, norm of estimates = 0.00010864867
Iteration 14, No. converged = 0, norm of estimates = 2.6760132e-05
Iteration 15, No. converged = 0, norm of estimates = 6.1411233e-06
Iteration 16, No. converged = 0, norm of estimates = 1.1174096e-06
Iteration 17, No. converged = 0, norm of estimates = 3.047356e-07
Iteration 18, No. converged = 1, norm of estimates = 5.6326848e-08
Iteration 19, No. converged = 2, norm of estimates = 1.9947734e-08
Iteration 20, No. converged = 2, norm of estimates = 3.935598e-09
Iteration 21, No. converged = 2, norm of estimates = 7.6414746e-10
Iteration 22, No. converged = 2, norm of estimates = 1.3783855e-10
Iteration 23, No. converged = 2, norm of estimates = 1.4348987e-11
Iteration 24, No. converged = 3, norm of estimates = 2.2715713e-12
Iteration 25, No. converged = 3, norm of estimates = 3.9695554e-13

```