F02BBF – NAG Fortran Library Routine Document

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

F02BBF calculates selected eigenvalues and eigenvectors of a real symmetric matrix by reduction to tridiagonal form, bisection and inverse iteration, where the selected eigenvalues lie within a given interval.

2 Specification

```
   SUBROUTINE F02BBF(A, IA, N, ALB, UB, M, MM, R, V, IV, D, E, E2, X,
  1                  G, C, ICOUNT, IFAIL)
   INTEGER          IA, N, M, MM, IV, ICOUNT(M), IFAIL
   real             A(IA,N), ALB, UB, R(M), V(IV,M), D(N), E(N),
  1                  E2(N), X(N,7), G(N)
   LOGICAL          C(N)
```

3 Description

The real symmetric matrix A is reduced to a symmetric tridiagonal matrix T by Householder's method. The eigenvalues which lie within a given interval $[l, u]$, are calculated by the method of bisection. The corresponding eigenvectors of T are calculated by inverse iteration. A back-transformation is then performed to obtain the eigenvectors of the original matrix A.

4 References

[1] Wilkinson J H and Reinsch C (1971) *Handbook for Automatic Computation II, Linear Algebra* Springer-Verlag

5 Parameters

1: A(IA,N) — **real** array   *Input/Output*

On entry: the lower triangle of the n by n symmetric matrix A. The elements of the array above the diagonal need not be set.

On exit: the elements of A below the diagonal are overwritten, and the rest of the array is unchanged.

2: IA — INTEGER   *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F02BBF is called.

Constraint: IA ≥ N.

3: N — INTEGER   *Input*

On entry: n, the order of the matrix A.

4: ALB — **real**   *Input*
5: UB — **real**   *Input*

On entry: l and u, the lower and upper end-points of the interval within which eigenvalues are to be calculated.

6: M — INTEGER   *Input*

On entry: an upper bound for the number of eigenvalues within the interval.

7: MM — INTEGER *Output*

On exit: the actual number of eigenvalues within the interval.

8: R(M) — *real* array *Output*

On exit: the eigenvalues, not necessarily in ascending order.

9: V(IV,M) — *real* array *Output*

On exit: the eigenvectors, stored by columns. The ith column corresponds to the ith eigenvalue. The eigenvectors are normalised so that the sum of the squares of the elements are equal to 1.

10: IV — INTEGER *Input*

On entry: the first dimension of the array V as declared in the (sub)program from which F02BBF is called.

Constraint: IV $\geq$ N.

11: D(N) — *real* array *Workspace*
12: E(N) — *real* array *Workspace*
13: E2(N) — *real* array *Workspace*
14: X(N,7) — *real* array *Workspace*
15: G(N) — *real* array *Workspace*
16: C(N) — LOGICAL array *Workspace*
17: ICOUNT(M) — INTEGER array *Output*

On exit: ICOUNT(i) contains the number of iterations for the ith eigenvalue.

18: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

M is less than the number of eigenvalues in the given interval. On exit MM contains the number of eigenvalues in the interval. Rerun with this value for M.

IFAIL = 2

More than 5 iterations are required to determine any one eigenvector.

7 Accuracy

There is no guarantee of the accuracy of the eigenvectors as the results depend on the original matrix and the multiplicity of the roots. For a detailed error analysis see Wilkinson and Reinsch [1] pp 222 and 436.

8 Further Comments

The time taken by the routine is approximately proportional to n^3.

This subroutine should only be used when less than 25% of the eigenvalues and the corresponding eigenvectors are required. Also this subroutine is less efficient with matrices which have multiple eigenvalues.

9   Example

To calculate the eigenvalues lying between -2.0 and 3.0, and the corresponding eigenvectors of the real symmetric matrix:

$$\begin{pmatrix} 0.5 & 0.0 & 2.3 & -2.6 \\ 0.0 & 0.5 & -1.4 & -0.7 \\ 2.3 & -1.4 & 0.5 & 0.0 \\ -2.6 & -0.7 & 0.0 & 0.5 \end{pmatrix}.$$

9.1   Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     F02BBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX, MMAX, IA, IV
      PARAMETER        (NMAX=8,MMAX=8,IA=NMAX,IV=NMAX)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             RLB, RUB
      INTEGER          I, IFAIL, J, M, MM, N
*     .. Local Arrays ..
      real             A(IA,NMAX), D(NMAX), E(NMAX), E2(NMAX), G(NMAX),
     +                 R(MMAX), V(IV,MMAX), X(NMAX,7)
      INTEGER          ICOUNT(MMAX)
      LOGICAL          C(NMAX)
*     .. External Subroutines ..
      EXTERNAL         F02BBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F02BBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, M
      WRITE (NOUT,*)
      IF (N.LT.1 .OR. N.GT.NMAX .OR. M.LT.1 .OR. M.GT.MMAX) THEN
         WRITE (NOUT,99999) 'N or M out of range: N = ', N, '  M = ', M
         STOP
      END IF
      READ (NIN,*) RLB, RUB, ((A(I,J),J=1,N),I=1,N)
      IFAIL = 1
*
      CALL F02BBF(A,IA,N,RLB,RUB,M,MM,R,V,IV,D,E,E2,X,G,C,ICOUNT,IFAIL)
*
      IF (IFAIL.NE.0) THEN
         WRITE (NOUT,99999) 'Error in F02BBF. IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,*) 'Eigenvalues'
         WRITE (NOUT,99998) (R(I),I=1,MM)
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Eigenvectors'
         DO 20 I = 1, N
            WRITE (NOUT,99998) (V(I,J),J=1,MM)
   20    CONTINUE
      END IF
      STOP
*
```

```
99999 FORMAT (1X,A,I5,A,I5)
99998 FORMAT (1X,8F9.4)
      END
```

9.2 Program Data

```
F02BBF Example Program Data
  4  3
 -2.0  3.0
  0.5  0.0  2.3 -2.6
  0.0  0.5 -1.4 -0.7
  2.3 -1.4  0.5  0.0
 -2.6 -0.7  0.0  0.5
```

9.3 Program Results

```
F02BBF Example Program Results

Eigenvalues
  -1.0000    2.0000

Eigenvectors
  -0.1000   -0.1000
  -0.7000   -0.7000
  -0.5000    0.5000
  -0.5000    0.5000
```