

NAG Library Routine Document

G02AAF

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

G02AAF computes the nearest correlation matrix, in the Frobenius norm, to a given square, input matrix.

2 Specification

```

SUBROUTINE G02AAF(G, LDG, N, ERRTOL, MAXITS, MAXIT, X, LDX, ITER, FEVAL,
1 NRMGRD, IFAIL)
      INTEGER          LDG, N, MAXITS, MAXIT, LDX, ITER, FEVAL, IFAIL
      double precision G(LDG,N), ERRTOL, X(LDX,N), NRMGRD

```

3 Description

A correlation matrix may be characterized as a real square matrix that is symmetric, has a unit diagonal and is positive semi-definite.

G02AAF applies an inexact Newton method to a dual formulation of the problem, as described by Qi and Sun (2006). It applies the improvements suggested by Borsdorf (2007).

4 References

Borsdorf R (2007) A Newton Algorithm for the Nearest Correlation Matrix. *M Sc Dissertation* School of Mathematics, University of Manchester

Qi H and Sun D (2006) A Quadratically Convergent Newton Method for Computing the Nearest Correlation Matrix *SIAM J. Matrix AnalAppl* **29(2)** 360–385

5 Parameters

- 1: G(LDG,N) – **double precision** array *Input/Output*
On entry: G , the initial matrix.
On exit: a symmetric matrix $\frac{1}{2}(G + G^T)$ with the diagonal set to I .
- 2: LDG – INTEGER *Input*
On entry: the first dimension of the array G as declared in the (sub)program from which G02AAF is called.
Constraint: $LDG \geq N$.
- 3: N – INTEGER *Input*
On entry: the size of the matrix G .
Constraint: $N > 0$.
- 4: ERRTOL – **double precision** *Input*
On entry: the termination tolerance for the Newton iteration. If $ERRTOL \leq 0.0$ then $n \times \sqrt{\text{machine precision}}$ is used.

- 5: MAXITS – INTEGER *Input*
On entry: MAXITS specifies the maximum number of iterations used for the iterative scheme used to solve the linear algebraic equations at each Newton step.
 If $\text{MAXITS} \leq 0$, $2 \times N$ is used.
- 6: MAXIT – INTEGER *Input*
On entry: specifies the maximum number of Newton iterations.
 If $\text{MAXIT} \leq 0$, 200 is used.
- 7: X(LDX,N) – *double precision* array *Output*
On exit: contains the nearest correlation matrix.
- 8: LDX – INTEGER *Input*
On entry: the first dimension of the array X as declared in the (sub)program from which G02AAF is called.
Constraint: $\text{LDX} \geq N$.
- 9: ITER – INTEGER *Output*
On exit: the number of Newton steps taken.
- 10: FEVAL – INTEGER *Output*
On exit: the number of function evaluations of the dual problem.
- 11: NRMGRD – *double precision* *Output*
On exit: the norm of the gradient of the last Newton step.
- 12: 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, $N \leq 0$,
 or $\text{LDG} < N$,
 or $\text{LDX} < N$.

IFAIL = 2

The routine fails to converge in MAXIT iterations. Increase MAXIT or check the call to the routine.

IFAIL = 3

Machine precision is limiting convergence. In this instance the returned value of X may be useful.

IFAIL = 4

An internal eigenproblem could not be solved. This should not occur. Please contact NAG with details of your call.

IFAIL = -999

Internal memory allocation failed.

7 Accuracy

The returned accuracy is controlled by ERRTOL and limited by *machine precision*.

8 Further Comments

None.

9 Example

This example finds the nearest correlation matrix to:

$$G = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}$$

9.1 Program Text

```
*      G02AAF Example Program Text
*      Mark 22 Release. NAG Copyright 2008.
*      .. Parameters ..
      INTEGER          NMAX, LDG, LDX, NOUT
      PARAMETER        (NMAX=4,LDG=5,LDX=NMAX,NOUT=6)
*      .. Local Scalars ..
      DOUBLE PRECISION ERRTOL, NRMGRD
      INTEGER          FEVAL, I, IFAIL, ITER, J, MAXIT, MAXITS, N
*      .. Local Arrays ..
      DOUBLE PRECISION G(LDG,NMAX), X(LDX,NMAX)
*      .. External Subroutines ..
      EXTERNAL         G02AAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'G02AAF Example Program Results'
      WRITE (NOUT,*)

*
*      Set up matrix G
      N = 4
      DO 40 J = 1, N
        DO 20 I = 1, N
          G(I,J) = 0.0
20      CONTINUE
        G(J,J) = 2.0D0
40      CONTINUE
        DO 60 J = 2, N
          G(J-1,J) = -1.0D0
          G(J,J-1) = -1.0D0
60      CONTINUE

*
*      Set up method parameters
      ERRTOL = 1.0D-7
      MAXITS = 200
      MAXIT = 10
*
```

```

      IFAIL = 1
      CALL G02AAF(G,LDG,N,ERRTOL,MAXITS,MAXIT,X,LDX,ITER,FEVAL,NRMGRD,
+              IFAIL)
*
      IF (IFAIL.EQ.0) THEN
        WRITE (NOUT,*) '      Nearest Correlation Matrix'
        WRITE (NOUT,99999) ((X(I,J),J=1,NMAX),I=1,NMAX)
        WRITE (NOUT,*)
        WRITE (NOUT,99998) ' Number of Newton steps taken:', ITER
        WRITE (NOUT,99997) ' Number of function evaluations:', FEVAL
        IF (NRMGRD.GT.ERRTOL) THEN
          WRITE (NOUT,99996) ' Norm of gradient of last Newton step:',
+              NRMGRD
        END IF
      ELSE
        WRITE (NOUT,99995) IFAIL
      END IF
      WRITE (NOUT,*)
*
99999 FORMAT (2X,4F11.5)
99998 FORMAT (A,I11)
99997 FORMAT (A,I9)
99996 FORMAT (A,E11.3)
99995 FORMAT (' ** G02AAF returned with IFAIL = ',I5)
      END

```

9.2 Program Data

None.

9.3 Program Results

G02AAF Example Program Results

Nearest Correlation Matrix			
1.00000	-0.80841	0.19159	0.10678
-0.80841	1.00000	-0.65623	0.19159
0.19159	-0.65623	1.00000	-0.80841
0.10678	0.19159	-0.80841	1.00000

Number of Newton steps taken:	3
Number of function evaluations:	4