NAG Fortran Library Routine Document G02BBF

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

G02BBF computes means and standard deviations of variables, sums of squares and cross-products of deviations from means, and Pearson product-moment correlation coefficients for a set of data omitting completely any cases with a missing observation for any variable.

2 Specification

```
SUBROUTINE GO2BBF(N, M, X, IX, MISS, XMISS, XBAR, STD, SSP, ISSP, R, IR, NCASES, IFAIL)

INTEGER

N, M, IX, MISS(M), ISSP, IR, NCASES, IFAIL

real

X(IX,M), XMISS(M), XBAR(M), STD(M), SSP(ISSP,M),

R(IR,M)
```

3 Description

The input data consist of n observations for each of m variables, given as an array

$$[x_{ij}], \quad i = 1, 2, \dots, n \ (n \ge 2), \ j = 1, 2, \dots, m \ (m \ge 2),$$

where x_{ij} is the *i*th observation on the *j*th variable. In addition, each of the *m* variables may optionally have associated with it a value which is to be considered as representing a missing observation for that variable; the missing value for the *j*th variable is denoted by xm_j . Missing values need not be specified for all variables.

Let $w_i = 0$ if observation i contains a missing value for any of those variables for which missing values have been declared, i.e., if $x_{ij} = xm_j$ for any j for which an xm_j has been assigned (see also Section 7); and $w_i = 1$ otherwise, for i = 1, 2, ..., n.

The quantities calculated are:

(a) Means:

$$\bar{x}_j = \frac{\sum_{i=1}^n w_i x_{ij}}{\sum_{i=1}^n w_i}, \quad j = 1, 2, \dots, m.$$

(b) Standard deviations:

$$s_j = \sqrt{\frac{\sum_{i=1}^n w_i (x_{ij} - \bar{x}_j)^2}{\sum_{i=1}^n w_i - 1}}, \quad j = 1, 2, \dots, m.$$

(c) Sums of squares and cross-products of deviations from means:

$$S_{jk} = \sum_{i=1}^{n} w_i (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k), \quad j, k = 1, 2, \dots, m.$$

(d) Pearson product-moment correlation coefficients:

$$R_{jk} = \frac{S_{jk}}{\sqrt{S_{jj}S_{kk}}}, \quad j, k = 1, 2, \dots, m.$$

If S_{ij} or S_{kk} is zero, R_{ik} is set to zero.

[NP3546/20A] G02BBF.1

4 References

None.

5 Parameters

1: N – INTEGER Input

On entry: the number, n, of observations or cases.

Constraint: $N \geq 2$.

2: M – INTEGER Input

On entry: the number, m, of variables.

Constraint: $M \ge 2$.

3: X(IX,M) - real array

Input

On entry: X(i, j) must be set to x_{ij} , the value of the *i*th observation on the *j*th variable, for i = 1, 2, ..., n; j = 1, 2, ..., m.

4: IX – INTEGER Input

On entry: the first dimension of the array X as declared in the (sub)program from which G02BBF is called.

Constraint: $IX \geq N$.

5: MISS(M) – INTEGER array

Input/Output

On entry: MISS(j) must be set equal to 1 if a missing value, xm_j , is to be specified for the jth variable in the array X, or set equal to 0 otherwise. Values of MISS must be given for all m variables in the array X.

On exit: The array MISS is overwritten by the routine, and the information it contained on entry is lost.

6: XMISS(M) – *real* array

Input/Output

On entry: XMISS(j) must be set to the missing value, xm_j , to be associated with the jth variable in the array X, for those variables for which missing values are specified by means of the array MISS (see Section 7).

On exit: The array XMISS is overwritten by the routine, and the information it contained on entry is lost.

7: XBAR(M) - real array

Output

On exit: the mean value, \bar{x}_j , of the jth variable, for j = 1, 2, ..., m.

8: STD(M) - real array

Output

On exit: the standard deviation, s_j , of the jth variable, for j = 1, 2, ..., m.

9: SSP(ISSP,M) – *real* array

Output

On exit: SSP(j,k) is the cross-product of deviations, S_{jk} , for $j,k=1,2,\ldots,m$.

10: ISSP - INTEGER

Input

On entry: the first dimension of the array SSP as declared in the (sub)program from which G02BBF is called.

Constraint: ISSP \geq M.

G02BBF.2 [NP3546/20A]

11: R(IR,M) - real array

Output

On exit: R(j,k) is the product-moment correlation coefficient, R_{jk} , between the jth and kth variables, for j, k = 1, 2, ..., m.

12: IR – INTEGER Input

On entry: the first dimension of the array R as declared in the (sub)program from which G02BBF is called.

Constraint: $IR \geq M$.

13: NCASES – INTEGER

Output

On exit: the number of cases actually used in the calculations (when cases involving missing values have been eliminated).

14: IFAIL – INTEGER

Input/Output

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 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, for users 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 < 2.

IFAIL = 2

On entry, M < 2.

IFAIL = 3

On entry, IX < N, or ISSP < M, or IR < M.

IFAIL = 4

After observations with missing values were omitted, no cases remained.

IFAIL = 5

After observations with missing values were omitted, only one case remained.

7 Accuracy

The routine does not use *additional precision* arithmetic for the accumulation of scalar products, so there may be a loss of significant figures for large n.

Users are warned of the need to exercise extreme care in their selection of missing values. The routine treats all values in the inclusive range $(1 \pm ACC) \times xm_j$, where xm_j is the missing value for variable j

[NP3546/20A] G02BBF.3

specified by the user, and ACC is a machine-dependent constant (see the Users' Note for your implementation) as missing values for variable j.

The user must therefore ensure that the missing value chosen for each variable is sufficiently different from all valid values for that variable so that none of the valid values fall within the range indicated above.

8 Further Comments

The time taken by the routine depends on n and m, and the occurrence of missing values.

The routine uses a two-pass algorithm.

9 Example

The following program reads in a set of data consisting of five observations on each of three variables. Missing values of 0.0 are declared for the first and third variables; no missing value is specified for the second variable. The means, standard deviations, sums of squares and cross-products of deviations from means, and Pearson product-moment correlation coefficients for all three variables are then calculated and printed, omitting completely all cases containing missing values; cases 3 and 4 are therefore eliminated, leaving only three cases in the calculations.

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.

```
GO2BBF Example Program Text
Mark 14 Revised. NAG Copyright 1989.
.. Parameters ..
INTEGER
                 M, N, IA, ISSP, ICORR
                 (M=3,N=5,IA=N,ISSP=M,ICORR=M)
PARAMETER
INTEGER
                NIN, NOUT
PARAMETER
                 (NIN=5,NOUT=6)
.. Local Scalars ..
INTEGER
                 I, IFAIL, J, NCASES
.. Local Arrays ..
real
                 A(IA,M), AMEAN(M), CORR(ICORR,M), SSP(ISSP,M),
                 STD(M), XMISS(M)
INTEGER
                 MISS(M)
.. External Subroutines ..
EXTERNAL
                 G02BBF
.. Executable Statements ..
WRITE (NOUT,*) 'G02BBF Example Program Results'
Skip heading in data file
READ (NIN, *)
READ (NIN,*) ((A(I,J),J=1,M),I=1,N)
WRITE (NOUT, *)
WRITE (NOUT, 99999) 'Number of variables (columns) =', M
WRITE (NOUT, 99999) 'Number of cases
                                      (rows)
WRITE (NOUT, *)
WRITE (NOUT,*) 'Data matrix is:-'
WRITE (NOUT, *)
WRITE (NOUT, 99998) (J, J=1, M)
WRITE (NOUT, 99997) (I, (A(I,J), J=1,M), I=1,N)
WRITE (NOUT, *)
Set up missing values before calling routine
MISS(1) = 1
MISS(2) = 0
MISS(3) = 1
XMISS(1) = 0.0e0
XMISS(3) = 0.0e0
IFAIL = 1
CALL GO2BBF(N,M,A,IA,MISS,XMISS,AMEAN,STD,SSP,ISSP,CORR,ICORR,
```

G02BBF.4 [NP3546/20A]

```
NCASES, IFAIL)
      IF (IFAIL.NE.O) THEN
         WRITE (NOUT, 99999) 'Routine fails, IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,*) 'Variable Mean
                                              St. dev.'
         WRITE (NOUT, 99996) (I, AMEAN(I), STD(I), I=1, M)
         WRITE (NOUT, *)
         WRITE (NOUT, *)
          'Sums of squares and cross-products of deviations'
         WRITE (NOUT, 99998) (I, I=1, M)
         WRITE (NOUT, 99997) (I, (SSP(I, J), J=1, M), I=1, M)
         WRITE (NOUT, *)
         WRITE (NOUT,*) 'Correlation coefficients'
         WRITE (NOUT, 99998) (I, I=1, M)
         WRITE (NOUT, 99997) (I, (CORR(I,J), J=1,M), I=1,M)
         WRITE (NOUT, *)
         WRITE (NOUT, 99999) 'Number of cases actually used: ', NCASES
      END IF
      STOP
99999 FORMAT (1X,A,I2)
99998 FORMAT (1x,6I12)
99997 FORMAT (1X, I3, 3F12.4)
99996 FORMAT (1X, 15, 2F11.4)
      END
```

9.2 Program Data

```
GO2BBF Example Program Data
              3.00
2.00
       3.00
4.00
         6.00
                 4.00
                 0.00
9.00
         9.00
0.00
         12.00
                 2.00
                5.00
12.00
         -1.00
```

9.3 Program Results

```
GO2BBF Example Program Results
Number of variables (columns) = 3
Number of cases
                   (rows) = 5
Data matrix is:-
          1 2
2.0000 3.0000
4.0000 6.0000
9.0000 9.0000
0.0000 12.0000
12.0000 -1.0000
             1
                                  3.0000
4.0000
0.0000
2.0000
5.0000
  1
  3
  4
         12.0000
  5
                       -1.0000
Variable Mean
                     St. dev.
                     5.2915
    1 6.0000
2 2.6667
                         3.5119
                       1.0000
          4.0000
Sums of squares and cross-products of deviations
                      2 3
-30.0000 10.0000
                        2
  1
         56.0000
        -30.0000 24.6667
10.0000 -4.0000
  2
                                      -4.0000
  3
                                      2.0000
Correlation coefficients
        1.0000 -0.8072 0.9449
-0.8072 1.0000 -0.5695
0.9449 -0.5695 1.0000
      1 2
  1
  2
  3
```

[NP3546/20A] G02BBF.5

Number of cases actually used: 3

G02BBF.6 (last) [NP3546/20A]