# NAG Fortran Library Routine Document

# G02HMF

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

G02HMF computes a robust estimate of the covariance matrix for user-supplied weight functions. The derivatives of the weight functions are not required.

# 2 Specification

SUBROUTINE GO2HMF(UCV, USERP, INDM, N, M, X, LDX, COV, A, WT, THETA, BL,1BD, MAXIT, NITMON, TOL, NIT, WK, IFAIL)INTEGERINDM, N, M, LDX, MAXIT, NITMON, NIT, IFAILrealUSERP(\*), X(LDX,M), COV(M\*(M+1)/2), A(M\*(M+1)/2),1WT(N), THETA(M), BL, BD, TOL, WK(2\*M)EXTERNALUCV

# **3** Description

For a set of n observations on m variables in a matrix X, a robust estimate of the covariance matrix, C, and a robust estimate of location,  $\theta$ , are given by

$$C = \tau^2 (A^T A)^{-1},$$

where  $\tau^2$  is a correction factor and A is a lower triangular matrix found as the solution to the following equations.

$$z_i = A(x_i - \theta)$$
$$\frac{1}{n} \sum_{i=1}^n w(\|z_i\|_2) z_i = 0$$

and

$$\frac{1}{n}\sum_{i=1}^{n}u(\|z_i\|_2)z_iz_i^T - v(\|z_i\|_2)I = 0,$$

where  $x_i$ , is a vector of length m containing the elements of the *i*th row of X,

 $z_i$  is a vector of length m,

I is the indentity matrix and 0 is the zero matrix.

and w, and u are suitable functions.

G02HMF covers two situations:

(i) 
$$v(t) = 1$$
 for all  $t$ ,

(ii) 
$$v(t) = u(t)$$
.

The robust covariance matrix may be calculated from a weighted sum of squares and cross-products matrix about  $\theta$  using weights  $wt_i = u(||z_i||)$ . In case (i) a divisor of n is used and in case (ii) a divisor of  $\sum_{i=1}^{n} wt_i$  is used. If  $w(.) = \sqrt{u(.)}$ , then the robust covariance matrix can be calculated by scaling each row of X by  $\sqrt{wt_i}$  and calculating an unweighted covariance matrix about  $\theta$ .

In order to make the estimate asymptotically unbiased under a Normal model a correction factor,  $\tau^2$ , is needed. The value of the correction factor will depend on the functions employed (see Huber (1981) and Marazzi (1987a)).

G02HMF finds A using the iterative procedure as given by Huber; see Huber (1981).

$$A_k = (S_k + I)A_{k-1}$$

and

$$\theta_{j_k} = \frac{b_j}{D_1} + \theta_{j_{k-1}}$$

where  $S_k = (s_{il})$ , for j, l = 1, 2, ..., m is a lower triangular matrix such that

$$s_{jl} = \begin{cases} -\min[\max(h_{jl}/D_2, -BL), BL], & j > l \\ \\ -\min[\max(\frac{1}{2}(h_{jj}/D_2 - 1), -BD), BD], & j = l \end{cases}$$

where

$$D_{1} = \sum_{i=1}^{n} w(||z_{i}||_{2})$$

$$D_{2} = \sum_{i=1}^{n} u(||z_{i}||_{2})$$

$$h_{jl} = \sum_{i=1}^{n} u(||z_{i}||_{2})z_{ij}z_{il}, \text{ for } j \ge l$$

$$b_{j} = \sum_{i=1}^{n} w(||z_{i}||_{2})(x_{ij} - b_{j})$$

and BD and BL are suitable bounds.

The value of  $\tau$  may be chosen so that C is unbiased if the observations are from a given distribution. G02HMF is based on routines in ROBETH; see Marazzi (1987a).

# 4 References

Huber P J (1981) Robust Statistics Wiley

Marazzi A (1987a) Weights for bounded influence regression in ROBETH Cah. Rech. Doc. IUMSP, No. 3 ROB 3 Institut Universitaire de Médecine Sociale et Préventive, Lausanne

## **5** Parameters

 1:
 UCV – SUBROUTINE, supplied by the user.
 External Procedure

UCV must return the values of the functions u and w for a given value of its argument. Its specification is:

```
SUBROUTINE UCV(T, USERP, U, W)
      real
                        T, USERP(*), U, W
      T – real
1:
                                                                                     Input
      On entry: the argument for which the functions u and w must be evaluated.
                                                                        External Procedure
2:
      USERP(*) - real array
The array USERP is included so that the user may pass parameter values to the routine UCV.
The values of USERP are not altered by G02HMF.
      U - real
3:
                                                                                    Output
      On exit: the value of the u function at the point T.
      Constraint: U \ge 0.0.
```

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4: W – <i>real</i>	Output
On exit: the value of the $w$ function at the point T.	
Constraint: $W \ge 0.0$ .	
UCV must be declared as EXTERNAL in the (sub)program from which Parameters denoted as <i>Input</i> must <b>not</b> be changed by this procedure.	G02HMF is called.

#### USERP(\*) - real array 2:

The array USERP is included so that the user may pass parameter values to the routine UCV. The values of USERP are not altered by G02HMF.

INDM - INTEGER 3:

On entry: indicates which form of the function v will be used.

If INDM = 1, v = 1. If INDM  $\neq 1$ , v = u.

N – INTEGER 4:

On entry: the number of observations, n.

Constraint: N > 1.

M – INTEGER 5:

On entry: the number of columns of the matrix X, i.e., number of independent variables, m.

*Constraint*:  $1 \le M \le N$ .

#### 6: X(LDX,M) - *real* array

On entry: X(i, j) must contain the *i*th observation on the *j*th variable, for i = 1, 2, ..., n;  $j = 1, 2, \ldots, m.$ 

#### 7: LDX - INTEGER

On entry: the first dimension of the array X as declared in the (sub)program from which G02HMF is called.

Constraint:  $LDX \ge N$ .

COV(M\*(M+1)/2) - real array8:

> On exit: a robust estimate of the covariance matrix, C. The upper triangular part of the matrix C is stored packed by columns (lower triangular stored by rows), that is  $C_{ij}$  is returned in  $COV(j \times (j-1)/2 + i), \ i \le j.$

A(M\*(M+1)/2) - real array 9:

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On entry: an initial estimate of the lower triangular real matrix A. Only the lower triangular elements must be given and these should be stored row-wise in the array.

The diagonal elements must be  $\neq 0$ , and in practice will usually be > 0. If the magnitudes of the columns of X are of the same order, the identity matrix will often provide a suitable initial value for A. If the columns of X are of different magnitudes, the diagonal elements of the initial value of Ashould be approximately inversely proportional to the magnitude of the columns of X.

*Constraint*:  $A(j \times (j-1)/2 + j) \neq 0.0$ , for j = 1, 2, ..., m.

On exit: the lower triangular elements of the inverse of the matrix A, stored row-wise.

User Workspace

# Input/Output

G02HMF.3

Input

Input

Input

Input

Input

Output

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10:	WT(N) - real array	Output
	On exit: WT(i) contains the weights, $wt_i = u(  z_i  _2)$ , for $i = 1, 2,, n$ .	
]	THETA(M) – <i>real</i> array	Input/Output
	On entry: an initial estimate of the location parameter, $\theta_j$ , for $j = 1, 2,,$	<i>m</i> .
	In many cases an initial estimate of $\theta_j = 0$ , for $j = 1, 2,, m$ , will be a medians may be used as given by G07DAF.	dequate. Alternatively
	On exit: THETA contains the robust estimate of the location parameter, $\theta_j$ ,	for $j = 1, 2,, m$ .
12:	BL – <i>real</i>	Input
	On entry: the magnitude of the bound for the off-diagonal elements of $S_k$ ,	BL.
	Suggested value: 0.9.	
	Constraint: $BL > 0.0$ .	
On Sug	BD – real	Input
	On entry: the magnitude of the bound for the diagonal elements of $S_k$ , BL	Э.
	Suggested value: 0.9.	
	Constraint: $BD > 0.0$ .	
	MAXIT – INTEGER	Input
	On entry: the maximum number of iterations that will be used during the o	calculation of A.
	Suggested value: 150.	
	Constraint: MAXIT $> 0$ .	
15:	NITMON – INTEGER	Input
	On entry: indicates the amount of information on the iteration that is printed	ed.
	If NITMON > 0, then the value of A, $\theta$ and $\delta$ (see Section 7) will be printe NITMON iterations.	ed at the first and every
	If NITMON $\leq$ 0, then no iteration monitoring is printed.	
	When printing occurs the output is directed to the current advisory message of	channel (See X04ABF.)
16:	TOL – <i>real</i>	Input
	On entry: the relative precision for the final estimate of the covariance mat when maximum $\delta$ (see Section 7) is less than TOL.	rix. Iteration will stop
	Constraint: $TOL > 0.0$ .	
17:	NIT – INTEGER	Output
	On exit: the number of iterations performed.	
18:	WK(2*M) – <i>real</i> array	Workspace
0.		Iranut/Outnut

IFAIL – INTEGER 19:

> 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

Input/Output

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

IFAIL = 2

On entry,	$TOL \leq 0.0$ ,
or	MAXIT $\leq 0$ ,
or	diagonal element of $A = 0.0$ ,
or	$BL \le 0.0,$
or	$BD \leq 0.0.$

#### IFAIL = 3

A column of X has a constant value.

#### IFAIL = 4

Value of U or W returned by the user-supplied subroutine UCV < 0.

#### IFAIL = 5

The routine has failed to converge in MAXIT iterations.

IFAIL = 6

Either the sum  $D_1$  or the sum  $D_2$  is zero. This may be caused by the functions u or w being too strict for the current estimate of A (or C). The user should either try a larger initial estimate of A or make the u and w functions less strict.

# 7 Accuracy

On successful exit the accuracy of the results is related to the value of TOL; see Section 5. At an iteration let

- (i) d1 = the maximum value of  $|s_{jl}|$
- (ii) d2 = the maximum absolute change in wt(i)
- (iii) d3 = the maximum absolute relative change in  $\theta_i$

and let  $\delta = \max(d1, d2, d3)$ . Then the iterative procedure is assumed to have converged when  $\delta < \text{TOL}$ .

### 8 Further Comments

The existence of A will depend upon the function u (see Marazzi (1987a)); also if X is not of full rank a value of A will not be found. If the columns of X are almost linearly related, then convergence will be slow.

If derivatives of the u and w functions are available then the method used in G02HLF will usually give much faster convergence.

[NP3546/20A]

# 9 Example

A sample of 10 observations on three variables is read in along with initial values for A and  $\theta$  and parameter values for the u and w functions,  $c_u$  and  $c_w$ . The covariance matrix computed by G02HMF is printed along with the robust estimate of  $\theta$ .

The subroutine UCV computes the Huber's weight functions:

$$u(t) = 1, \quad \text{if} \quad t \le c_u^2$$
$$u(t) = \frac{c_u}{t^2}, \quad \text{if} \quad t > c_u^2$$
$$w(t) = 1, \quad \text{if} \quad t \le c_w$$
$$w(t) = \frac{c_w}{t}, \quad \text{if} \quad t > c_w.$$

and

### 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.

```
GO2HMF Example Program Text
*
      Mark 14 Release. NAG Copyright 1989.
*
*
      .. Parameters ..
      INTEGER
                        NIN, NOUT
      PARAMETER
                        (NIN=5,NOUT=6)
                        NMAX, MMAX, LDX
      INTEGER
                        (NMAX=10,MMAX=3,LDX=NMAX)
      PARAMETER
      .. Local Scalars ..
*
      real
                        BD, BL, TOL
                        I, IFAIL, INDM, J, K, L1, L2, M, MAXIT, MM, N,
      INTEGER
                        NIT, NITMON
      .. Local Arrays ..
*
                        A(MMAX*(MMAX+1)/2), COV(MMAX*(MMAX+1)/2),
THETA(MMAX), USERP(2), WK(MMAX*(MMAX+1)/2),
     real
     +
     +
                        WT(NMAX), X(LDX,MMAX)
      .. External Subroutines ..
                       GO2HMF, UCV, XO4ABF
      EXTERNAL
      .. Executable Statements ..
      WRITE (NOUT, *) 'GO2HMF Example Program Results'
      Skip heading in data file
      READ (NIN,*)
      CALL X04ABF(1,NOUT)
      Read in the dimensions of X
      READ (NIN,*) N, M
      IF (N.GT.O .AND. N.LE.NMAX .AND. M.GT.O .AND. M.LE.MMAX) THEN
         Read in the X matrix
÷
         DO 20 I = 1, N
            READ (NIN, \star) (X(I,J), J=1, M)
   20
         CONTINUE
         Read in the initial value of A
*
         MM = ((M+1)*M)/2
         READ (NIN, \star) (A(J), J=1, MM)
         Read in the initial value of THETA
         READ (NIN,*) (THETA(J),J=1,M)
         Read in the values of the parameters of the ucv functions
*
         READ (NIN,*) USERP(1), USERP(2)
         Set the values remaining parameters
*
         INDM = 1
         BL = 0.9e0
         BD = 0.9e0
         MAXIT = 50
         TOL = 0.5e-4
         * Change NITMON to a positive value if monitoring information
*
           is required *
         NITMON = 0
```

```
IFAIL = 0
*
         CALL GO2HMF(UCV, USERP, INDM, N, M, X, LDX, COV, A, WT, THETA, BL, BD,
     ^{+}
                      MAXIT, NITMON, TOL, NIT, WK, IFAIL)
*
         WRITE (NOUT, *)
         WRITE (NOUT, 99999) 'GO2HMF required ', NIT,
           ' iterations to converge'
     +
         WRITE (NOUT, *)
         WRITE (NOUT, *) 'Robust covariance matrix'
         L2 = 0
         DO 40 J = 1, M
            L1 = L2 + 1
            L2 = L2 + J
            WRITE (NOUT, 99998) (COV(K), K=L1, L2)
   40
         CONTINUE
         WRITE (NOUT, *)
         WRITE (NOUT, *) 'Robust estimates of THETA'
         DO 60 J = 1, M
            WRITE (NOUT, 99997) THETA(J)
   60
        CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,A,I4,A)
99998 FORMAT (1X,6F10.3)
99997 FORMAT (1X,F10.3)
      END
*
      SUBROUTINE UCV(T,USERP,U,W)
*
      .. Scalar Arguments ..
      real
                     т, U, W
      .. Array Arguments ..
*
      real
                     USERP(2)
      .. Local Scalars ..
      real
                     СU, СW, Т2
      .. Executable Statements ..
      u function
+
      CU = USERP(1)
      U = 1.0e0
      IF (T.NE.O) THEN
         T2 = T*T
         IF (T2.GT.CU) U = CU/T2
      END IF
      w function
*
      CW = USERP(2)
      IF (T.GT.CW) THEN
         W = CW/T
      ELSE
        W = 1.0e0
      END IF
      END
```

#### 9.2 Program Data

GO2HMF Example Program Data : N M 10 3 3.4 6.9 12.2 : X1 X2 X3 6.4 2.5 15.1 4.9 5.5 14.2 7.3 1.9 18.2 8.8 3.6 11.7 8.4 1.3 17.9 5.3 3.1 15.0 2.7 8.1 7.7 6.1 3.0 21.9 5.3 2.2 13.9 : End of X1 X2 and X3 values 1.0 0.0 1.0 0.0 0.0 1.0 : A 0.0 0.0 0.0 : THETA 4.0 2.0 : CU CW

# 9.3 Program Results

GO2HMF Example Program Results GO2HMF required 34 iterations to converge Robust covariance matrix 3.278 -3.692 5.284 4.739 -6.409 11.837 Robust estimates of THETA 5.700 3.864 14.704