# NAG C Library Function Document nag robust m corr user fn (g02hlc)

## 1 Purpose

nag\_robust\_m\_corr\_user\_fn (g02hlc) calculates a robust estimate of the covariance matrix for user-supplied weight functions and their derivatives.

## 2 Specification

## 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:

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

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

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

where  $x_i$  is a vector of length m containing the elements of the ith row of X,

 $z_i$  is a vector of length m,

I is the identity matrix and 0 is the zero matrix,

and w and u are suitable functions.

nag\_robust\_m\_corr\_user\_fn (g02hlc) 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)).

nag robust m corr user fn (g02hlc) finds A using the iterative procedure as given by Huber.

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

and

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

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

$$s_{jl} = \begin{cases} -\min[\max(h_{jl}/D_3, -BL), BL], & j > l \\ -\min[\max((h_{jj}/(2D_3 - D_4/D_2)), -BD), BD], & j = l \end{cases}$$

where

$$D_{1} = \sum_{i=1}^{n} \left\{ w(\|z_{i}\|_{2}) + \frac{1}{m} w'(\|z_{i}\|_{2}) \|z_{i}\|_{2} \right\}$$

$$D_{2} = \sum_{i=1}^{n} \left\{ \frac{1}{p} (u'(\|z_{i}\|_{2}) \|z_{i}\|_{2} + 2u(\|z_{i}\|_{2})) \|z_{i}\|_{2} - v'(\|z_{i}\|_{2}) \right\} \|z_{i}\|_{2}$$

$$D_{3} = \frac{1}{m+2} \sum_{i=1}^{n} \left\{ \frac{1}{m} (u'(\|z_{i}\|_{2}) \|z_{i}\|_{2} + 2u(\|z_{i}\|_{2})) + u(\|z_{i}\|_{2}) \right\} \|z_{i}\|_{2}^{2}$$

$$D_{4} = \sum_{i=1}^{n} \left\{ \frac{1}{m} u(\|z_{i}\|_{2}) \|z_{i}\|_{2}^{2} - v(\|z_{i}\|_{2}^{2}) \right\}$$

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

$$h_{jj} = \sum_{i=1}^{n} u(\|z_{i}\|_{2}) \left(z_{ij}^{2} - \|z_{ij}\|_{2}^{2} / m\right)$$

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

and BD and BL are suitable bounds.

nag robust m corr user fn (g02hlc) 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 Arguments

1: **order** – Nag\_OrderType

Input

On entry: the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = **Nag\_RowMajor**. See Section 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this argument.

Constraint: order = Nag RowMajor or Nag ColMajor.

g02hlc.2 [NP3660/8]

2: **ucv** – function, supplied by the user

External Function

**ucv** must return the values of the functions u and w and their derivatives for a given value of its argument.

Its specification is:

void ucv (double t, double \*u, double \*ud, double \*w, double \*wd, Nag\_Comm \*comm)

1:  $\mathbf{t}$  – double

Input

On entry: the argument for which the functions u and w must be evaluated.

2: **u** – double \*

Output

On exit: the value of the u function at the point t.

3: **ud** – double \*

Output

On exit: the value of the derivative of the u function at the point t.

4:  $\mathbf{w}$  – double \*

Output

On exit: the value of the w function at the point t.

5: **wd** – double \*

Output

On exit: the value of the derivative of the w function at the point t.

6: **comm** – Nag Comm \*

Communication Structure

Pointer to structure of type Nag\_Comm; the following members are relevant to ucv.

user - double \*

iuser - Integer \*

**p** – Pointer

The type Pointer will be void \*. Before calling nag\_robust\_m\_corr\_user\_fn (g02hlc) these pointers may be allocated memory by the user and initialized with various quantities for use by **ucv** when called from nag\_robust\_m\_corr\_user\_fn (g02hlc).

3: **indm** – Integer

Input

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

indm = 1

v = 1.

indm  $\neq 1$ 

v = u.

4:  $\mathbf{n}$  – Integer

Input

On entry: n, the number of observations.

Constraint:  $\mathbf{n} > 1$ .

5: m - Integer

Input

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

Constraint:  $1 \leq m \leq n$ .

[NP3660/8]

6:  $\mathbf{x}[dim]$  – const double

Input

Note: the dimension, dim, of the array x must be at least

```
max(1, pdx \times m) when order = Nag\_ColMajor; max(1, n \times pdx) when order = Nag\_RowMajor.
```

Where  $\mathbf{X}(i,j)$  appears in this document, it refers to the array element

```
if order = Nag_ColMajor, \mathbf{x}[(j-1) \times \mathbf{pdx} + i - 1]; if order = Nag_RowMajor, \mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1].
```

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

7:  $\mathbf{pdx}$  - Integer Input

On entry: the stride separating matrix row or column elements (depending on the value of **order**) in the array  $\mathbf{x}$ .

Constraints:

```
if order = Nag_ColMajor, pdx \ge n; if order = Nag_RowMajor, pdx \ge m.
```

8:  $\mathbf{cov}[dim] - \mathbf{double}$ 

Output

**Note**: the dimension, dim, of the array cov must be at least  $\mathbf{m} \times (\mathbf{m} + 1)/2$ .

On exit: contains 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),  $C_{ij}$  is returned in  $\mathbf{cov}(j \times (j-1)/2+i)$ ,  $i \le j$ .

9:  $\mathbf{a}[dim]$  – double

Input/Output

**Note**: the dimension, dim, of the array **a** must be at least  $\mathbf{m} \times (\mathbf{m} + 1)/2$ .

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 A should be approximately inversely proportional to the magnitude of the columns of X.

Constraint:  $\mathbf{a}[j \times (j-1)/2 + j] \neq 0.0$ , for j = 0, 1, ..., m-1.

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

10:  $\mathbf{wt}[\mathbf{n}]$  – double

Output

On exit:  $\mathbf{wt}[i-1]$  contains the weights,  $wt_i = u(||z_i||_2)$ , for  $i = 1, 2, \dots, n$ .

11:  $\mathbf{theta}[\mathbf{m}] - \mathbf{double}$ 

Input/Output

On entry: an initial estimate of the location argument,  $\theta_i$ , for  $j = 1, 2, \dots, m$ .

In many cases an initial estimate of  $\theta_j = 0$ , for j = 1, 2, ..., m, will be adequate. Alternatively medians may be used as given by nag\_median\_1var (g07dac).

On exit: contains the robust estimate of the location argument,  $\theta_i$ , for  $i = 1, 2, \dots, m$ .

12: **bl** – double

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.

g02hlc.4 [NP3660/8]

## 13: **bd** – double *Input*

On entry: the magnitude of the bound for the diagonal elements of  $S_k$ , BD.

Suggested value: 0.9.

Constraint: bd > 0.0.

#### 14: **maxit** – Integer

Input

On entry: the maximum number of iterations that will be used during the 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.

#### nitmon > 0

The value of A,  $\theta$  and  $\delta$  (see Section 7) will be printed at the first and every **nitmon** iterations.

#### $nitmon \leq 0$

No iteration monitoring is printed.

#### 16: **outfile** – const char \*

Input

On entry: a null terminated character string giving the name of the file to which results should be printed. If **outfile** = **NULL** or an empty string then the stdout stream is used. Note that the file will be opened in the append mode.

## 17: **tol** – double

Input

On entry: the relative precision for the final estimates of the covariance matrix. Iteration will stop when maximum  $\delta$  (see Section 7) is less than **tol**.

Constraint: tol > 0.0.

## 18: **nit** – Integer \*

Output

On exit: the number of iterations performed.

#### 19: **comm** – Nag Comm \*

Communication Structure

The NAG communication argument (see Section 2.2.1.1 of the Essential Introduction).

## 20: **fail** – NagError \*

Input/Output

The NAG error argument (see Section 2.6 of the Essential Introduction).

## 6 Error Indicators and Warnings

#### NE ALLOC FAIL

Dynamic memory allocation failed.

#### **NE BAD PARAM**

On entry, argument (value) had an illegal value.

## **NE CONST COL**

Column  $\langle value \rangle$  of **x** has constant value.

## **NE\_CONVERGENCE**

Iterations to calculate weights failed to converge.

### NE FUN RET VAL

```
u value returned by \mathbf{ucv} < 0.0: u(\langle value \rangle) = \langle value \rangle. w value returned by \mathbf{ucv} < 0.0: w(\langle value \rangle) = \langle value \rangle.
```

## NE INT

```
On entry, \mathbf{m} = \langle value \rangle.
Constraint: \mathbf{m} \geq 1.
On entry, \mathbf{maxit} = \langle value \rangle.
Constraint: \mathbf{maxit} > 0.
On entry, \mathbf{n} = \langle value \rangle.
Constraint: \mathbf{n} > 1.
On entry, \mathbf{pdx} = \langle value \rangle.
Constraint: \mathbf{pdx} > 0.
```

## NE\_INT\_2

```
On entry, \mathbf{m} = \langle value \rangle, \mathbf{n} = \langle value \rangle.
Constraint: 1 \leq \mathbf{m} \leq \mathbf{n}.
On entry, \mathbf{n} = \langle value \rangle, \mathbf{m} = \langle value \rangle.
Constraint: \mathbf{n} \geq \mathbf{m}.
On entry, \mathbf{pdx} = \langle value \rangle, \mathbf{m} = \langle value \rangle.
Constraint: \mathbf{pdx} \geq \mathbf{m}.
On entry, \mathbf{pdx} = \langle value \rangle, \mathbf{n} = \langle value \rangle.
Constraint: \mathbf{pdx} \geq \mathbf{n}.
```

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

## NE\_NOT\_CLOSE\_FILE

Cannot close file \(\langle value \rangle \).

### NE NOT WRITE FILE

Cannot open file \( \nabla value \rangle \) for writing.

### **NE REAL**

```
On entry, \mathbf{bd} = \langle value \rangle. Constraint: \mathbf{bd} > 0.0. On entry, \mathbf{bl} = \langle value \rangle. Constraint: \mathbf{bl} > 0.0. On entry, \mathbf{tol} = \langle value \rangle. Constraint: \mathbf{tol} > 0.0.
```

## NE\_ZERO\_DIAGONAL

On entry, diagonal element  $\langle value \rangle$  of **a** is 0.0.

g02hlc.6 [NP3660/8]

## NE\_ZERO\_SUM

The sum D1 is zero.

The sum D2 is zero.

The sum D3 is zero.

## 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  $|s_{il}|$
- (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.

## 9 Example

A sample of 10 observations on three variables is read in along with initial values for A and **theta** and argument values for the u and w functions,  $c_u$  and  $c_w$ . The covariance matrix computed by nag\_robust\_m\_corr\_user\_fn (g02hlc) is printed along with the robust estimate of  $\theta$ . The function **ucv** computes the Huber's weight functions:

$$u(t) = 1$$
, if  $t \le c_u^2$ 

$$u(t) = \frac{c_u}{t^2}, \quad \text{if} \quad t > c_u^2$$

and

$$w(t) = 1$$
, if  $t \le c_w$ 

$$w(t) = \frac{c_w}{t}$$
, if  $t > c_w$ 

and their derivatives.

## 9.1 Program Text

```
/* Scalars */
  double bd, bl, tol;
  Integer exit_status, i__, indm, j, k, 11, 12, m, maxit, mm, n, nit, nitmon;
  Integer pdx;
  NagError fail;
  Nag_OrderType order;
  Nag_Comm comm;
  /* Arrays */
  double *a=0, *cov=0, *theta=0, *userp=0, *wt=0, *x=0;
#ifdef NAG_COLUMN_MAJOR
#define X(I,J) \times [(J-1) * pdx + I - 1]
  order = Nag_ColMajor;
#else
#define X(I,J) \times [(I-1) * pdx + J - 1]
 order = Nag_RowMajor;
#endif
  INIT_FAIL(fail);
  exit_status = 0;
  Vprintf("nag_robust_m_corr_user_fn (g02hlc) Example Program Results\n");
  /* Skip heading in data file */
Vscanf("%*[^\n] ");
  /* Read in the dimensions of X */
  Vscanf("%ld%ld%*[^\n] ", &n, &m);
  /* Allocate memory */
  if ( !(a = NAG\_ALLOC(m*(m+1)/2, double)) | |
       !(cov = NAG\_ALLOC(m*(m+1)/2, double)) | |
       !(theta = NAG_ALLOC(m, double)) ||
       !(userp = NAG_ALLOC(2, double)) ||
       !(wt = NAG_ALLOC(n, double)) ||
       !(x = NAG\_ALLOC(n * m, double)))
      Vprintf("Allocation failure\n");
      exit_status = -1;
      goto END;
#ifdef NAG_COLUMN_MAJOR
  pdx = n;
#else
 pdx = m;
#endif
  /* Read in the X matrix */
  for (i__ = 1; i__ <= n; ++i__)
      for (j = 1; j <= m; ++j)
  Vscanf("%lf", &X(i__,j));</pre>
      Vscanf("%*[^\n] ");
   }
  /* Read in the initial value of A */
  mm = (m + 1) * m / 2;
  for (j = 1; j \le mm; ++j)
  Vscanf("%lf", &a[j - 1]);
Vscanf("%*[^\n] ");
  /* Read in the initial value of theta */
  for (j = 1; j \le m; ++j)
  Vscanf("%lf", &theta[j - 1]);
Vscanf("%*[^\n] ");
  /* Read in the values of the parameters of the ucv functions */
  Vscanf("%lf%lf%*[^\n] ", &userp[0], &userp[1]);
  /\star Set the values of remaining parameters \star/
  indm = 1;
```

g02hlc.8 [NP3660/8]

```
b1 = 0.9;
 bd = 0.9;
 maxit = 50;
 tol = 5e-5;
 /* Change nitmon to a positive value if monitoring information
             is required
  */
 nitmon = 0;
 comm.p = (void *)userp;
 /* nag_robust_m_corr_user_fn (g02hlc).
  * Calculates a robust estimation of a correlation matrix,
   * user-supplied weight function plus derivatives
  * /
 nag_robust_m_corr_user_fn(order, ucv, indm, n, m, x, pdx, cov, a, wt,
                             theta, bl, bd, maxit, nitmon, 0, tol, &nit, &comm,
                             &fail);
  if (fail.code != NE_NOERROR)
      Vprintf("Error from nag_robust_m_corr_user_fn (g02hlc).\n%s\n",
              fail.message);
      exit_status = 1;
      goto END;
 Vprintf("\n");
 Vprintf("nag_robust_m_corr_user_fn (g02hlc) required %4ld "
          "iterations to converge\n\n", nit);
 Vprintf("Robust covariance matrix\n");
 1\bar{2} = 0;
 for (j = 1; j \le m; ++j)
      11 = 12 + 1;
      12 += j;
      for (k = 11; k \le 12; ++k)
        Vprintf("%10.3f%s", cov[k - 1], k%6 == 0 | | k == 12 ?"\n":" ");
 Vprintf("\n");
 Vprintf("Robust estimates of theta\n");
 for (j = 1; j <= m; ++j)
    Vprintf(" %10.3f\n", theta[j - 1]);</pre>
END:
 if (a) NAG_FREE(a);
 if (cov) NAG_FREE(cov);
 if (theta) NAG_FREE(theta);
 if (userp) NAG_FREE(userp);
 if (wt) NAG_FREE(wt);
 if (x) NAG_FREE(x);
 return exit_status;
static void ucv(double t, double *u, double *ud, double *wd, double *wd,
                Naq_Comm *comm)
                  double t2, cu, cw;
                  double *userp = (double *)comm->p;
                   /* Function Body */
                  cu = userp[0];
                  *u = 1.0;
                   *ud = 0.0;
                   if (t != 0.0)
                     {
                       t2 = t * t;
                       if (t2 > cu)
                         {
                           *u = cu / t2;
                           *ud = *u * -2.0 / t;
```

```
}
}
/* w function and derivative */
cw = userp[1];
if (t > cw)
{
    *w = cw / t;
    *wd = -(*w) / t;
}
else
{
    *w = 1.0;
    *wd = 0.0;
}
return;
}
```

## 9.2 Program Data

### 9.3 Program Results

```
nag_robust_m_corr_user_fn (g02hlc) Example Program Results
nag_robust_m_corr_user_fn (g02hlc) required 25 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
```

g02hlc.10 (last) [NP3660/8]