# **NAG Library Routine Document**

#### G07DBF

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

G07DBF computes an M-estimate of location with (optional) simultaneous estimation of the scale using Huber's algorithm.

### 2 Specification

## 3 Description

The data consists of a sample of size n, denoted by  $x_1, x_2, \ldots, x_n$ , drawn from a random variable X.

The  $x_i$  are assumed to be independent with an unknown distribution function of the form

$$F((x_i - \theta)/\sigma)$$

where  $\theta$  is a location parameter, and  $\sigma$  is a scale parameter. M-estimators of  $\theta$  and  $\sigma$  are given by the solution to the following system of equations:

$$\sum_{i=1}^{n} \psi\left(\left(x_{i} - \hat{\theta}\right)/\hat{\sigma}\right) = 0 \tag{1}$$

$$\sum_{i=1}^{n} \chi\left(\left(x_i - \hat{\theta}\right)/\hat{\sigma}\right) = (n-1)\beta \tag{2}$$

where  $\psi$  and  $\chi$  are given functions, and  $\beta$  is a constant, such that  $\hat{\sigma}$  is an unbiased estimator when  $x_i$ , for  $i=1,2,\ldots,n$  has a Normal distribution. Optionally, the second equation can be omitted and the first equation is solved for  $\hat{\theta}$  using an assigned value of  $\sigma=\sigma_c$ .

The values of  $\psi\left(\frac{x_i-\hat{\theta}}{\hat{\sigma}}\right)\hat{\sigma}$  are known as the Winsorized residuals.

The following functions are available for  $\psi$  and  $\chi$  in G07DBF.

#### (a) Null Weights

$$\psi(t) = t \qquad \qquad \chi(t) = \frac{t^2}{2}$$

Use of these null functions leads to the mean and standard deviation of the data.

#### (b) Huber's Function

$$\psi(t) = \max(-c, \min(c, t))$$

$$\chi(t) = \frac{\|t\|^2}{2} \|t\| \le d$$

$$\chi(t) = \frac{d^2}{2} \|t\| > d$$

### (c) Hampel's Piecewise Linear Function

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$$\psi_{h_1,h_2,h_3}(t) = -\psi_{h_1,h_2,h_3}(-t)$$

$$\psi_{h_1,h_2,h_3}(t) = t$$
  $0 \le t \le h_1$   $\chi(t) = \frac{|t|^2}{2}|t| \le d$ 

$$\psi_{h_1,h_2,h_3}(t) = h_1 \qquad h_1 \le t \le h_2$$

$$\psi_{h_1,h_2,h_3}(t) = h_1(h_3 - t)/(h_3 - h_2) \qquad h_2 \le t \le h_3 \qquad \chi(t) = \frac{d^2}{2}|t| > d$$

$$\psi_{h_1,h_2,h_3}(t) = 0 t > h_3$$

#### (d) Andrew's Sine Wave Function

$$\psi(t) = \sin t \qquad -\pi \le t \le \pi \qquad \chi(t) = \frac{|t|^2}{2} |t| \le d$$

$$\psi(t) = 0 \qquad \text{otherwise} \qquad \chi(t) = \frac{d^2}{2} |t| > d$$

#### (e) Tukey's Bi-weight

$$\psi(t) = t\left(1 - t^2\right)^2 \qquad |t| \le 1 \qquad \qquad \chi(t) = \frac{|t|^2}{2}|t| \le d$$

$$\psi(t) = t\left(1 - t^2\right)^2 = 0 \qquad \text{otherwise} \qquad \chi(t) = \frac{d^2}{2}|t| > d$$

where c,  $h_1$ ,  $h_2$ ,  $h_3$  and d are constants.

Equations (1) and (2) are solved by a simple iterative procedure suggested by Huber:

$$\hat{\sigma}_k = \sqrt{\frac{1}{\beta(n-1)} \left( \sum_{i=1}^n \chi \left( \frac{x_i - \hat{\theta}_{k-1}}{\hat{\sigma}_{k-1}} \right) \right) \hat{\sigma}_{k-1}^2}$$

and

$$\hat{\theta}_k = \hat{\theta}_{k-1} + \frac{1}{n} \sum_{i=1}^n \psi\left(\frac{x_i - \hat{\theta}_{k-1}}{\hat{\sigma}_k}\right) \hat{\sigma}_k$$

or

$$\hat{\sigma}_k = \sigma_c$$
, if  $\sigma$  is fixed.

The initial values for  $\hat{\theta}$  and  $\hat{\sigma}$  may either be user-supplied or calculated within G07DBF as the sample median and an estimate of  $\sigma$  based on the median absolute deviation respectively.

G07DBF is based upon subroutine LYHALG within the ROBETH library, see Marazzi (1987).

#### 4 References

Hampel F R, Ronchetti E M, Rousseeuw P J and Stahel W A (1986) Robust Statistics. The Approach Based on Influence Functions Wiley

Huber P J (1981) Robust Statistics Wiley

Marazzi A (1987) Subroutines for robust estimation of location and scale in ROBETH *Cah. Rech. Doc. IUMSP, No. 3 ROB 1* Institut Universitaire de Médecine Sociale et Préventive, Lausanne

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#### 5 Parameters

#### 1: ISIGMA – INTEGER

Input

On entry: the value assigned to ISIGMA determines whether  $\hat{\sigma}$  is to be simultaneously estimated.

ISIGMA = 0

The estimation of  $\hat{\sigma}$  is bypassed and SIGMA is set equal to  $\sigma_c$ .

ISIGMA = 1

 $\hat{\sigma}$  is estimated simultaneously.

2: N – INTEGER

On entry: n, the number of observations.

Constraint: N > 1.

3: X(N) - REAL (KIND=nag wp) array

Input

Input

On entry: the vector of observations,  $x_1, x_2, \ldots, x_n$ .

4: IPSI – INTEGER Input

On entry: which  $\psi$  function is to be used.

$$\begin{aligned} \text{IPSI} &= 0 \\ \psi(t) &= t. \end{aligned}$$

IPSI = 1

Huber's function.

IPSI = 2

Hampel's piecewise linear function.

IPSI = 3

Andrew's sine wave,

IPSI = 4

Tukey's bi-weight.

#### 5: C - REAL (KIND=nag wp)

Input

On entry: if IPSI = 1, C must specify the parameter, c, of Huber's  $\psi$  function. C is not referenced if IPSI  $\neq$  1.

Constraint: if IPSI = 1, C > 0.0.

6:  $H1 - REAL (KIND=nag_wp)$ 

Input

7: H2 – REAL (KIND=nag wp)

Input

8: H3 – REAL (KIND=nag\_wp)

Input

On entry: if IPSI = 2, H1, H2 and H3 must specify the parameters,  $h_1$ ,  $h_2$ , and  $h_3$ , of Hampel's piecewise linear  $\psi$  function. H1, H2 and H3 are not referenced if IPSI  $\neq$  2.

Constraint: 0 < H1 < H2 < H3 and H3 > 0.0 if IPSI = 2.

9: DCHI – REAL (KIND=nag wp)

Input

On entry: d, the parameter of the  $\chi$  function. DCHI is not referenced if IPSI = 0.

Constraint: if IPSI  $\neq 0$ , DCHI > 0.0.

10: THETA - REAL (KIND=nag wp)

Input/Output

On entry: if SIGMA > 0 then THETA must be set to the required starting value of the estimation of the location parameter  $\hat{\theta}$ . A reasonable initial value for  $\hat{\theta}$  will often be the sample mean or median.

On exit: the M-estimate of the location parameter,  $\hat{\theta}$ .

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### 11: SIGMA - REAL (KIND=nag\_wp)

Input/Output

On entry: the role of SIGMA depends on the value assigned to ISIGMA, as follows:

if ISIGMA = 1, SIGMA must be assigned a value which determines the values of the starting points for the calculations of  $\hat{\theta}$  and  $\hat{\sigma}$ . If SIGMA  $\leq$  0.0 then G07DBF will determine the starting points of  $\hat{\theta}$  and  $\hat{\sigma}$ . Otherwise the value assigned to SIGMA will be taken as the starting point for  $\hat{\sigma}$ , and THETA must be assigned a value before entry, see above;

if ISIGMA = 0, SIGMA must be assigned a value which determines the value of  $\sigma_c$ , which is held fixed during the iterations, and the starting value for the calculation of  $\hat{\theta}$ . If SIGMA  $\leq$  0, then G07DBF will determine the value of  $\sigma_c$  as the median absolute deviation adjusted to reduce bias (see G07DAF) and the starting point for  $\hat{\theta}$ . Otherwise, the value assigned to SIGMA will be taken as the value of  $\sigma_c$  and THETA must be assigned a relevant value before entry, see above.

On exit: contains the M-estimate of the scale parameter,  $\hat{\sigma}$ , if ISIGMA was assigned the value 1 on entry, otherwise SIGMA will contain the initial fixed value  $\sigma_c$ .

12: MAXIT – INTEGER

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

Suggested value: MAXIT = 50.

Constraint: MAXIT > 0.

#### 13: TOL – REAL (KIND=nag\_wp)

Input

Input

*On entry*: the relative precision for the final estimates. Convergence is assumed when the increments for THETA, and SIGMA are less than  $TOL \times max(1.0, \sigma_{k-1})$ .

Constraint: TOL > 0.0.

14:  $RS(N) - REAL (KIND=nag_wp) array$ 

Output

On exit: the Winsorized residuals.

15: NIT – INTEGER Output

On exit: the number of iterations that were used during the estimation.

16: WRK(N) - REAL (KIND=nag wp) array

Output

On exit: if SIGMA  $\leq 0.0$  on entry, WRK will contain the n observations in ascending order.

17: 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.

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.

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

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### 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 1,
                 MAXIT < 0,
      or
                 TOL \leq 0.0,
      or
                 ISIGMA \neq 0 or 1,
      or
                 IPSI < 0,
      or
                 IPSI > 4.
      or
IFAIL = 2
      On entry, C \le 0.0 and IPSI = 1,
                 H1 < 0.0 and IPSI = 2,
                 H1 = H2 = H3 = 0.0 and IPSI = 2,
      or
      or
                 H1 > H2 and IPSI = 2,
                 H1 > H3 and IPSI = 2,
      or
                 H2 > H3 and IPSI = 2,
      or
                 DCHI \leq 0.0 and IPSI \neq 0.
      or
```

On entry, all elements of the input array X are equal.

```
IFAIL = 4
```

IFAIL = 3

SIGMA, the current estimate of  $\sigma$ , is zero or negative. This error exit is very unlikely, although it may be caused by too large an initial value of SIGMA.

```
IFAIL = 5
```

The number of iterations required exceeds MAXIT.

```
IFAIL = 6
```

On completion of the iterations, the Winsorized residuals were all zero. This may occur when using the ISIGMA = 0 option with a redescending  $\psi$  function, i.e., Hampel's piecewise linear function, Andrew's sine wave, and Tukey's biweight.

If the given value of  $\sigma$  is too small, then the standardized residuals  $\frac{x_i - \hat{\theta}_k}{\sigma_c}$ , will be large and all the residuals may fall into the region for which  $\psi(t) = 0$ . This may incorrectly terminate the iterations thus making THETA and SIGMA invalid.

Re-enter the routine with a larger value of  $\sigma_c$  or with ISIGMA = 1.

#### 7 Accuracy

On successful exit the accuracy of the results is related to the value of TOL, see Section 5.

#### **8** Further Comments

When you supply the initial values, care has to be taken over the choice of the initial value of  $\sigma$ . If too small a value of  $\sigma$  is chosen then initial values of the standardized residuals  $\frac{x_i - \hat{\theta}_k}{\sigma}$  will be large. If the redescending  $\psi$  functions are used, i.e., Hampel's piecewise linear function, Andrew's sine wave, or Tukey's bi-weight, then these large values of the standardized residuals are Winsorized as zero. If a

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sufficient number of the residuals fall into this category then a false solution may be returned, see page 152 of Hampel *et al.* (1986).

# 9 Example

The following program reads in a set of data consisting of eleven observations of a variable X.

For this example, Hampel's Piecewise Linear Function is used (IPSI = 2), values for  $h_1$ ,  $h_2$  and  $h_3$  along with d for the  $\chi$  function, being read from the data file.

Using the following starting values various estimates of  $\theta$  and  $\sigma$  are calculated and printed along with the number of iterations used:

- (a) G07DBF determines the starting values,  $\sigma$  is estimated simultaneously.
- (b) You must supply the starting values,  $\sigma$  is estimated simultaneously.
- (c) G07DBF determines the starting values,  $\sigma$  is fixed.
- (d) You must supply the starting values,  $\sigma$  is fixed.

### 9.1 Program Text

```
Program g07dbfe
     GO7DBF Example Program Text
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1
      .. Use Statements .
     Use nag_library, Only: g07dbf, nag_wp
      .. Implicit None Statement ..
!
     Implicit None
!
      .. Parameters ..
                                       :: nin = 5, nout = 6
     Integer, Parameter
      .. Local Scalars ..
!
                                       :: c, dchi, h1, h2, h3, sigma, sigsav, &
     Real (Kind=nag_wp)
                                          thesav, theta, tol
                                       :: ifail, ipsi, isigma, maxit, n, nit
     Integer
!
      .. Local Arrays ..
     Real (Kind=nag_wp), Allocatable :: rs(:), wrk(:), x(:)
!
      .. Executable Statements ..
     Write (nout,*) 'GO7DBF Example Program Results'
     Write (nout,*)
     Skip heading in data file
!
     Read (nin,*)
!
     Read in the problem size
     Read (nin,*) n
     Allocate (x(n),rs(n),wrk(n))
     Read in data
     Read (nin,*) x(1:n)
     Read in details of algorithm to use
     Read (nin,*) ipsi, dchi, maxit
     If (ipsi==2) Then
       Read (nin,*) h1, h2, h3
     End If
     Display titles
     Write (nout,*) '
                               Input parameters
                                                     Output parameters'
     Write (nout,*) 'ISIGMA SIGMA THETA TOL
                                                    SIGMA THETA'
d_lp: Do
        Read (nin,*,Iostat=ifail) isigma, sigma, theta, tol
        If (ifail/=0) Then
```

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```
Exit d_lp
End If

! Save the input parameters for later display
    sigsav = sigma
    thesav = theta
! Compute M-estimates
    ifail = 0
    Call g07dbf(isigma,n,x,ipsi,c,h1,h2,h3,dchi,theta,sigma,maxit,tol,rs, &
        nit,wrk,ifail)
! Display results
    Write (nout,99999) isigma, sigsav, thesav, tol, sigma, theta
    End Do d_lp

99999 Format (1X,I3,3X,2F8.4,F7.4,F9.4,F8.4,I4)
    End Program g07dbfe
```

#### 9.2 Program Data

```
GO7DBF Example Program Data
11
                                              :: N
13.0 11.0 16.0 5.0 3.0 18.0
 9.0 8.0 6.0 27.0 7.0
                                             :: End of X
:: IPSI,DCHI,MAXIT
 2 1.5 50
1.5 3.0 4.5
                                             :: H1,H2,H3
                                        :: ISIGMA, SIGMA, THETA, TOL
          -1.0
                     0.0 0.0001
  1
                     2.0 0.0001
0.0 0.0001
  1
            7.0
           -1.0
  \cap
           7.0
                      2.0 0.0001
```

#### 9.3 Program Results

GO7DBF Example Program Results

	Input	parameters		Output parameters	
ISIGMA	SIGMA	THETA	TOL	SIGMA	THETA
1	-1.0000	0.0000	0.0001	6.3247	10.5487
1	7.0000	2.0000	0.0001	6.3249	10.5487
0	-1.0000	0.0000	0.0001	5.9304	10.4896
0	7.0000	2.0000	0.0001	7.0000	10.6500

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