

# NAG Library Routine Document

## G07BEF

**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

G07BEF computes maximum likelihood estimates for arguments of the Weibull distribution from data which may be right-censored.

### 2 Specification

```

SUBROUTINE G07BEF (CENS, N, X, IC, BETA, GAMMA, TOL, MAXIT, SEBETA,      &
                  SEGAM, CORR, DEV, NIT, WK, IFAIL)
INTEGER           N, IC(*), MAXIT, NIT, IFAIL
REAL (KIND=nag_wp) X(N), BETA, GAMMA, TOL, SEBETA, SEGAM, CORR, DEV,  &
                  WK(N)
CHARACTER(1)     CENS

```

### 3 Description

G07BEF computes maximum likelihood estimates of the arguments of the Weibull distribution from exact or right-censored data.

For  $n$  realizations,  $y_i$ , from a Weibull distribution a value  $x_i$  is observed such that

$$x_i \leq y_i.$$

There are two situations:

- (a) exactly specified observations, when  $x_i = y_i$
- (b) right-censored observations, known by a lower bound, when  $x_i < y_i$ .

The probability density function of the Weibull distribution, and hence the contribution of an exactly specified observation to the likelihood, is given by:

$$f(x; \lambda, \gamma) = \lambda \gamma x^{\gamma-1} \exp(-\lambda x^\gamma), \quad x > 0, \quad \text{for } \lambda, \gamma > 0;$$

while the survival function of the Weibull distribution, and hence the contribution of a right-censored observation to the likelihood, is given by:

$$S(x; \lambda, \gamma) = \exp(-\lambda x^\gamma), \quad x > 0, \quad \text{for } \lambda, \gamma > 0.$$

If  $d$  of the  $n$  observations are exactly specified and indicated by  $i \in D$  and the remaining  $(n - d)$  are right-censored, then the likelihood function,  $\text{Like}(\lambda, \gamma)$  is given by

$$\text{Like}(\lambda, \gamma) \propto (\lambda \gamma)^d \left( \prod_{i \in D} x_i^{\gamma-1} \right) \exp \left( -\lambda \sum_{i=1}^n x_i^\gamma \right).$$

To avoid possible numerical instability a different parameterisation  $\beta, \gamma$  is used, with  $\beta = \log(\lambda)$ . The kernel log-likelihood function,  $L(\beta, \gamma)$ , is then:

$$L(\beta, \gamma) = d \log(\gamma) + d\beta + (\gamma - 1) \sum_{i \in D} \log(x_i) - e^\beta \sum_{i=1}^n x_i^\gamma.$$

If the derivatives  $\frac{\partial L}{\partial \beta}$ ,  $\frac{\partial L}{\partial \gamma}$ ,  $\frac{\partial^2 L}{\partial \beta^2}$ ,  $\frac{\partial^2 L}{\partial \beta \partial \gamma}$  and  $\frac{\partial^2 L}{\partial \gamma^2}$  are denoted by  $L_1$ ,  $L_2$ ,  $L_{11}$ ,  $L_{12}$  and  $L_{22}$ , respectively, then the maximum likelihood estimates,  $\hat{\beta}$  and  $\hat{\gamma}$ , are the solution to the equations:

$$L_1(\hat{\beta}, \hat{\gamma}) = 0 \quad (1)$$

and

$$L_2(\hat{\beta}, \hat{\gamma}) = 0 \quad (2)$$

Estimates of the asymptotic standard errors of  $\hat{\beta}$  and  $\hat{\gamma}$  are given by:

$$\text{se}(\hat{\beta}) = \sqrt{\frac{-L_{22}}{L_{11}L_{22} - L_{12}^2}}, \quad \text{se}(\hat{\gamma}) = \sqrt{\frac{-L_{11}}{L_{11}L_{22} - L_{12}^2}}.$$

An estimate of the correlation coefficient of  $\hat{\beta}$  and  $\hat{\gamma}$  is given by:

$$\frac{L_{12}}{\sqrt{L_{11}L_{22}}}.$$

**Note:** if an estimate of the original argument  $\lambda$  is required, then

$$\hat{\lambda} = \exp(\hat{\beta}) \quad \text{and} \quad \text{se}(\hat{\lambda}) = \hat{\lambda} \text{se}(\hat{\beta}).$$

The equations (1) and (2) are solved by the Newton–Raphson iterative method with adjustments made to ensure that  $\hat{\gamma} > 0.0$ .

## 4 References

Gross A J and Clark V A (1975) *Survival Distributions: Reliability Applications in the Biomedical Sciences* Wiley

Kalbfleisch J D and Prentice R L (1980) *The Statistical Analysis of Failure Time Data* Wiley

## 5 Arguments

- 1: CENS – CHARACTER(1) *Input*  
*On entry:* indicates whether the data is censored or non-censored.  
 CENS = 'N'  
 Each observation is assumed to be exactly specified. IC is not referenced.  
 CENS = 'C'  
 Each observation is censored according to the value contained in IC(*i*), for  $i = 1, 2, \dots, n$ .  
*Constraint:* CENS = 'N' or 'C'.
- 2: N – INTEGER *Input*  
*On entry:*  $n$ , the number of observations.  
*Constraint:*  $N \geq 1$ .
- 3: X(N) – REAL (KIND=nag\_wp) array *Input*  
*On entry:* X(*i*) contains the *i*th observation,  $x_i$ , for  $i = 1, 2, \dots, n$ .  
*Constraint:* X(*i*) > 0.0, for  $i = 1, 2, \dots, n$ .
- 4: IC(\*) – INTEGER array *Input*  
**Note:** the dimension of the array IC must be at least N if CENS = 'C', and at least 1 otherwise.  
*On entry:* if CENS = 'C', then IC(*i*) contains the censoring codes for the *i*th observation, for  $i = 1, 2, \dots, n$ .

If  $IC(i) = 0$ , the  $i$ th observation is exactly specified.

If  $IC(i) = 1$ , the  $i$ th observation is right-censored.

If  $CENS = 'N'$ , then  $IC$  is not referenced.

*Constraint:* if  $CENS = 'C'$ , then  $IC(i) = 0$  or  $1$ , for  $i = 1, 2, \dots, n$ .

- 5: BETA – REAL (KIND=nag\_wp) Output  
*On exit:* the maximum likelihood estimate,  $\hat{\beta}$ , of  $\beta$ .
- 6: GAMMA – REAL (KIND=nag\_wp) Input/Output  
*On entry:* indicates whether an initial estimate of  $\gamma$  is provided.  
 If  $GAMMA > 0.0$ , it is taken as the initial estimate of  $\gamma$  and an initial estimate of  $\beta$  is calculated from this value of  $\gamma$ .  
 If  $GAMMA \leq 0.0$ , then initial estimates of  $\gamma$  and  $\beta$  are calculated, internally, providing the data contains at least two distinct exact observations. (If there are only two distinct exact observations, then the largest observation must not be exactly specified.) See Section 9 for further details.  
*On exit:* contains the maximum likelihood estimate,  $\hat{\gamma}$ , of  $\gamma$ .
- 7: TOL – REAL (KIND=nag\_wp) Input  
*On entry:* the relative precision required for the final estimates of  $\beta$  and  $\gamma$ . Convergence is assumed when the absolute relative changes in the estimates of both  $\beta$  and  $\gamma$  are less than TOL.  
 If  $TOL = 0.0$ , then a relative precision of 0.000005 is used.  
*Constraint:* **machine precision**  $\leq TOL \leq 1.0$  or  $TOL = 0.0$ .
- 8: MAXIT – INTEGER Input  
*On entry:* the maximum number of iterations allowed.  
 If  $MAXIT \leq 0$ , then a value of 25 is used.
- 9: SEBETA – REAL (KIND=nag\_wp) Output  
*On exit:* an estimate of the standard error of  $\hat{\beta}$ .
- 10: SEGAM – REAL (KIND=nag\_wp) Output  
*On exit:* an estimate of the standard error of  $\hat{\gamma}$ .
- 11: CORR – REAL (KIND=nag\_wp) Output  
*On exit:* an estimate of the correlation between  $\hat{\beta}$  and  $\hat{\gamma}$ .
- 12: DEV – REAL (KIND=nag\_wp) Output  
*On exit:* the maximized kernel log-likelihood,  $L(\hat{\beta}, \hat{\gamma})$ .
- 13: NIT – INTEGER Output  
*On exit:* the number of iterations performed.

14: WK(N) – REAL (KIND=nag\_wp) array *Workspace*

15: IFAIL – INTEGER *Input/Output*

*On entry:* IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation 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 argument, 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).

## 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, CENS  $\neq$  'N' or 'C',  
 or  $N < 1$ ,  
 or  $TOL < 0.0$ ,  
 or  $0.0 < TOL < \textit{machine precision}$ ,  
 or  $TOL > 1.0$ .

IFAIL = 2

On entry, the  $i$ th observation,  $X(i) \leq 0.0$ , for some  $i = 1, 2, \dots, n$ ,  
 or the  $i$ th censoring code,  $IC(i) \neq 0$  or 1, for some  $i = 1, 2, \dots, n$  and CENS = 'C'.

IFAIL = 3

On entry, there are no exactly specified observations, or the routine was requested to calculate initial values and there are either less than two distinct exactly specified observations or there are exactly two and the largest observation is one of the exact observations.

IFAIL = 4

The method has failed to converge in MAXIT iterations. You should increase TOL or MAXIT.

IFAIL = 5

Process has diverged. The process is deemed divergent if three successive increments of  $\beta$  or  $\gamma$  increase or if the Hessian matrix of the Newton–Raphson process is singular. Either different initial estimates should be provided or the data should be checked to see if the Weibull distribution is appropriate.

IFAIL = 6

A potential overflow has been detected. This is an unlikely exit usually caused by a large input estimate of  $\gamma$ .

IFAIL = -99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

Given that the Weibull distribution is a suitable model for the data and that the initial values are reasonable the convergence to the required accuracy, indicated by TOL, should be achieved.

## 8 Parallelism and Performance

G07BEF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

## 9 Further Comments

The initial estimate of  $\gamma$  is found by calculating a Kaplan–Meier estimate of the survival function,  $\hat{S}(x)$ , and estimating the gradient of the plot of  $\log(-\log(\hat{S}(x)))$  against  $x$ . This requires the Kaplan–Meier estimate to have at least two distinct points.

The initial estimate of  $\hat{\beta}$ , given a value of  $\hat{\gamma}$ , is calculated as

$$\hat{\beta} = \log \left( \frac{d}{\sum_{i=1}^n x_i^{\hat{\gamma}}} \right).$$

## 10 Example

In a study, 20 patients receiving an analgesic to relieve headache pain had the following recorded relief times (in hours):

1.1 1.4 1.3 1.7 1.9 1.8 1.6 2.2 1.7 2.7 4.1 1.8 1.5 1.2 1.4 3.0 1.7 2.3 1.6 2.0

(See Gross and Clark (1975).) This data is read in and a Weibull distribution fitted assuming no censoring; the parameter estimates and their standard errors are printed.

### 10.1 Program Text

```

Program g07befe
!      G07BEF Example Program Text
!      Mark 26 Release. NAG Copyright 2016.
!
!      .. Use Statements ..
!      Use nag_library, Only: g07bef, nag_wp
!      .. Implicit None Statement ..
!      Implicit None
!      .. Parameters ..

```

```

Integer, Parameter      :: nin = 5, nout = 6
! .. Local Scalars ..
Real (Kind=nag_wp)      :: beta, corr, dev, gamma, sebeta,      &
                        segam, tol
Integer                 :: ifail, lic, maxit, n, nit
Character (1)           :: cens
! .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: wk(:), x(:)
Integer, Allocatable    :: ic(:)
! .. Executable Statements ..
Write (nout,*) 'G07BEF Example Program Results'
Write (nout,*)

! Skip heading in data file
Read (nin,*)

! Read in the problem size and control parameters
Read (nin,*) cens, n, tol, maxit

If (cens=='N' .Or. cens=='n') Then
  lic = 0
Else
  lic = n
End If
Allocate (x(n),ic(lic),wk(n))

! Read in data
Read (nin,*) x(1:n)

! Read in censor flag if required
If (lic>0) Then
  Read (nin,*) ic(1:n)
End If

! Read in initial estimate of GAMMA
Read (nin,*) gamma

! Calculate estimates
ifail = 0
Call g07bef(cens,n,x,ic,beta,gamma,tol,maxit,sebeta,segam,corr,dev,nit, &
wk,ifail)

! Display results
Write (nout,99999) ' BETA = ', beta, ' Standard error = ', sebeta
Write (nout,99999) ' GAMMA = ', gamma, ' Standard error = ', segam

99999 Format (1X,2(A,F10.4))
End Program g07befe

```

## 10.2 Program Data

```

G07BEF Example Program Data
'N' 20 0.0 0      :: CENS,N,TOL,MAXIT
1.1 1.4 1.3 1.7 1.9
1.8 1.6 2.2 1.7 2.7
4.1 1.8 1.5 1.2 1.4
3.0 1.7 2.3 1.6 2.0      :: End of X
0.0                  :: GAMMA (initial estimate are calculated from data)

```

## 10.3 Program Results

G07BEF Example Program Results

```

BETA =      -2.1073 Standard error =      0.4627
GAMMA =      2.7870 Standard error =      0.4273

```

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