

NAG Library Routine Document

G10ACF

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

G10ACF estimates the values of the smoothing parameter and fits a cubic smoothing spline to a set of data.

2 Specification

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SUBROUTINE G10ACF (METHOD, WEIGHT, N, X, Y, WT, YHAT, C, LDC, RSS, DF,      &
                  RES, H, CRIT, RHO, U, TOL, MAXCAL, WK, IFAIL)
INTEGER          N, LDC, MAXCAL, IFAIL
REAL (KIND=nag_wp) X(N), Y(N), WT(*), YHAT(N), C(LDC,3), RSS, DF,      &
                  RES(N), H(N), CRIT, RHO, U, TOL, WK(7*(N+2))
CHARACTER(1)    METHOD, WEIGHT

```

3 Description

For a set of n observations (x_i, y_i) , for $i = 1, 2, \dots, n$, the spline provides a flexible smooth function for situations in which a simple polynomial or nonlinear regression model is not suitable.

Cubic smoothing splines arise as the unique real-valued solution function f , with absolutely continuous first derivative and squared-integrable second derivative, which minimizes

$$\sum_{i=1}^n w_i (y_i - f(x_i))^2 + \rho \int_{-\infty}^{\infty} (f''(x))^2 dx,$$

where w_i is the (optional) weight for the i th observation and ρ is the smoothing parameter. This criterion consists of two parts: the first measures the fit of the curve and the second the smoothness of the curve. The value of the smoothing parameter ρ weights these two aspects; larger values of ρ give a smoother fitted curve but, in general, a poorer fit. For details of how the cubic spline can be fitted see Hutchinson and de Hoog (1985) and Reinsch (1967).

The fitted values, $\hat{y} = (\hat{y}_1, \hat{y}_2, \dots, \hat{y}_n)^T$, and weighted residuals, r_i , can be written as:

$$\hat{y} = Hy \quad \text{and} \quad r_i = \sqrt{w_i}(y_i - \hat{y}_i)$$

for a matrix H . The residual degrees of freedom for the spline is $\text{trace}(I - H)$ and the diagonal elements of H are the leverages.

The parameter ρ can be estimated in a number of ways.

- (i) The degrees of freedom for the spline can be specified, i.e., find ρ such that $\text{trace}(H) = \nu_0$ for given ν_0 .
- (ii) Minimize the cross-validation (CV), i.e., find ρ such that the CV is minimized, where

$$\text{CV} = \frac{1}{\sum_{i=1}^n w_i} \sum_{i=1}^n \left[\frac{r_i}{1 - h_{ii}} \right]^2.$$

- (iii) Minimize the generalized cross-validation (GCV), i.e., find ρ such that the GCV is minimized, where

$$\text{GCV} = \frac{n^2}{\sum_{i=1}^n w_i} \left[\frac{\sum_{i=1}^n r_i^2}{\left(\sum_{i=1}^n (1 - h_{ii}) \right)^2} \right].$$

G10ACF requires the x_i to be strictly increasing. If two or more observations have the same x_i value then they should be replaced by a single observation with y_i equal to the (weighted) mean of the y values and weight, w_i , equal to the sum of the weights. This operation can be performed by G10ZAF.

The algorithm is based on Hutchinson (1986). C05AZF is used to solve for ρ given ν_0 and the method of E04ABF/E04ABA is used to minimize the GCV or CV.

4 References

Hastie T J and Tibshirani R J (1990) *Generalized Additive Models* Chapman and Hall

Hutchinson M F (1986) Algorithm 642: A fast procedure for calculating minimum cross-validation cubic smoothing splines *ACM Trans. Math. Software* **12** 150–153

Hutchinson M F and de Hoog F R (1985) Smoothing noisy data with spline functions *Numer. Math.* **47** 99–106

Reinsch C H (1967) Smoothing by spline functions *Numer. Math.* **10** 177–183

5 Parameters

1: METHOD – CHARACTER(1) *Input*

On entry: indicates whether the smoothing parameter is to be found by minimization of the CV or GCV functions, or by finding the smoothing parameter corresponding to a specified degrees of freedom value.

METHOD = 'C'

Cross-validation is used.

METHOD = 'D'

The degrees of freedom are specified.

METHOD = 'G'

Generalized cross-validation is used.

Constraint: METHOD = 'C', 'D' or 'G'.

2: WEIGHT – CHARACTER(1) *Input*

On entry: indicates whether user-defined weights are to be used.

WEIGHT = 'W'

User-defined weights should be supplied in WT.

WEIGHT = 'U'

The data is treated as unweighted.

Constraint: WEIGHT = 'W' or 'U'.

3: N – INTEGER *Input*

On entry: n , the number of observations.

Constraint: $N \geq 3$.

- 4: X(N) – REAL (KIND=nag_wp) array Input
On entry: the distinct and ordered values x_i , for $i = 1, 2, \dots, n$.
Constraint: $X(i) < X(i + 1)$, for $i = 1, 2, \dots, n - 1$.
- 5: Y(N) – REAL (KIND=nag_wp) array Input
On entry: the values y_i , for $i = 1, 2, \dots, n$.
- 6: WT(*) – REAL (KIND=nag_wp) array Input
Note: the dimension of the array WT must be at least N if WEIGHT = 'W'.
On entry: if WEIGHT = 'W', WT must contain the n weights. Otherwise WT is not referenced and unit weights are assumed.
Constraint: if WEIGHT = 'W', $WT(i) > 0.0$, for $i = 1, 2, \dots, n$.
- 7: YHAT(N) – REAL (KIND=nag_wp) array Output
On exit: the fitted values, \hat{y}_i , for $i = 1, 2, \dots, n$.
- 8: C(LDC, 3) – REAL (KIND=nag_wp) array Output
On exit: the spline coefficients. More precisely, the value of the spline approximation at t is given by $((C(i, 3) \times d + C(i, 2)) \times d + C(i, 1)) \times d + \hat{y}_i$, where $x_i \leq t < x_{i+1}$ and $d = t - x_i$.
- 9: LDC – INTEGER Input
On entry: the first dimension of the array C as declared in the (sub)program from which G10ACF is called.
Constraint: $LDC \geq N - 1$.
- 10: RSS – REAL (KIND=nag_wp) Output
On exit: the (weighted) residual sum of squares.
- 11: DF – REAL (KIND=nag_wp) Output
On exit: the residual degrees of freedom. If METHOD = 'D' this will be $n - \text{CRIT}$ to the required accuracy.
- 12: RES(N) – REAL (KIND=nag_wp) array Output
On exit: the (weighted) residuals, r_i , for $i = 1, 2, \dots, n$.
- 13: H(N) – REAL (KIND=nag_wp) array Output
On exit: the leverages, h_{ii} , for $i = 1, 2, \dots, n$.
- 14: CRIT – REAL (KIND=nag_wp) Input/Output
On entry: if METHOD = 'D', the required degrees of freedom for the spline.
 If METHOD = 'C' or 'G', CRIT need not be set.
Constraint: $2.0 < \text{CRIT} \leq N$.
On exit: if METHOD = 'C', the value of the cross-validation, or if METHOD = 'G', the value of the generalized cross-validation function, evaluated at the value of ρ returned in RHO.
- 15: RHO – REAL (KIND=nag_wp) Output
On exit: the smoothing parameter, ρ .

- 16: U – REAL (KIND=nag_wp) Input
On entry: the upper bound on the smoothing parameter. If $U \leq \text{TOL}$, $U = 1000.0$ will be used instead. See Section 9 for details on how this parameter is used.
- 17: TOL – REAL (KIND=nag_wp) Input
On entry: the accuracy to which the smoothing parameter RHO is required. TOL should preferably be not much less than $\sqrt{\epsilon}$, where ϵ is the *machine precision*. If $\text{TOL} < \epsilon$, $\text{TOL} = \sqrt{\epsilon}$ will be used instead.
- 18: MAXCAL – INTEGER Input
On entry: the maximum number of spline evaluations to be used in finding the value of ρ . If $\text{MAXCAL} < 3$, $\text{MAXCAL} = 100$ will be used instead.
- 19: WK($7 \times (N + 2)$) – REAL (KIND=nag_wp) array Workspace
- 20: 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).

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, CRIT = $\langle \text{value} \rangle$.
Constraint: if METHOD = 'D', $\text{CRIT} > 2.0$.
- On entry, CRIT = $\langle \text{value} \rangle$.
Constraint: if METHOD = 'D', $\text{CRIT} \leq N$.
- On entry, LDC = $\langle \text{value} \rangle$ and $N = \langle \text{value} \rangle$.
Constraint: $\text{LDC} \geq N - 1$.
- On entry, METHOD is not valid: METHOD = $\langle \text{value} \rangle$.
- On entry, N = $\langle \text{value} \rangle$.
Constraint: $N \geq 3$.
- On entry, WEIGHT is not valid: WEIGHT = $\langle \text{value} \rangle$.

IFAIL = 2

- On entry, at least one element of WT ≤ 0.0 .

IFAIL = 3

- On entry, X is not a strictly ordered array.

IFAIL = 4

For the specified degrees of freedom, $RHO > U$: $U = \langle value \rangle$.

IFAIL = 5

Accuracy of TOL cannot be achieved: $TOL = \langle value \rangle$.

IFAIL = 6

MAXCAL iterations have been performed.

IFAIL = 7

Optimum value of RHO lies above U: $U = \langle value \rangle$.

IFAIL = -99

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

See Section 3.8 in the Essential Introduction for further information.

IFAIL = -399

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

See Section 3.7 in the Essential Introduction for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.6 in the Essential Introduction for further information.

7 Accuracy

When minimizing the cross-validation or generalized cross-validation, the error in the estimate of ρ should be within $\pm 3(TOL \times RHO + TOL)$. When finding ρ for a fixed number of degrees of freedom the error in the estimate of ρ should be within $\pm 2 \times TOL \times \max(1, RHO)$.

Given the value of ρ , the accuracy of the fitted spline depends on the value of ρ and the position of the x values. The values of $x_i - x_{i-1}$ and w_i are scaled and ρ is transformed to avoid underflow and overflow problems.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The time to fit the spline for a given value of ρ is of order n .

When finding the value of ρ that gives the required degrees of freedom, the algorithm examines the interval 0.0 to U. For small degrees of freedom the value of ρ can be large, as in the theoretical case of two degrees of freedom when the spline reduces to a straight line and ρ is infinite. If the CV or GCV is to be minimized then the algorithm searches for the minimum value in the interval 0.0 to U. If the function is decreasing in that range then the boundary value of U will be returned. In either case, the larger the value of U the more likely is the interval to contain the required solution, but the process will be less efficient.

Regression splines with a small ($< n$) number of knots can be fitted by E02BAF and E02BEF.

10 Example

This example uses the data given by Hastie and Tibshirani (1990), which consists of the age, x_i , and C-peptide concentration (pmol/ml), y_i , from a study of the factors affecting insulin-dependent diabetes mellitus in children. The data is input, reduced to a strictly ordered set by G10ZAF and a spline with 5 degrees of freedom is fitted by G10ACF. The fitted values and residuals are printed.

10.1 Program Text

```

Program g10acfe

!      G10ACF Example Program Text

!      Mark 25 Release. NAG Copyright 2014.

!      .. Use Statements ..
Use nag_library, Only: g10acf, g10zaf, nag_wp
!      .. Implicit None Statement ..
Implicit None
!      .. Parameters ..
Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
Real (Kind=nag_wp)         :: crit, df, rho, rss, tol, u
Integer                    :: i, ifail, ldc, lwk, lwt, maxcal, n, &
                          nord
Character (1)              :: method, weight
!      .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: c(:, :), h(:), res(:), wk(:), wt(:), &
                          wwt(:), x(:), xord(:), y(:), &
                          yhat(:), yord(:)
Integer, Allocatable       :: iwrk(:)
!      .. Executable Statements ..
Write (nout,*) 'G10ACF Example Program Results'
Write (nout,*)

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

If (weight=='W' .Or. weight=='w') Then
  lwt = n
Else
  lwt = 0
End If
ldc = n - 1
lwk = 7*(n+2)
Allocate (x(n),y(n),wt(lwt),xord(n),yord(n),wwt(n),yhat(n),c(ldc,3), &
  res(n),h(n),wk(lwk),iwrk(n))

!      Read in data
If (lwt>0) Then
  Read (nin,*)(x(i),y(i),wt(i),i=1,n)
Else
  Read (nin,*)(x(i),y(i),i=1,n)
End If

!      Read in control parameters
Read (nin,*) u, tol, maxcal, crit

!      Sort data, removing ties and weighting accordingly
ifail = 0
Call g10zaf(weight,n,x,y,wt,nord,xord,yord,wwt,rss,iwrk,ifail)

!      Fit cubic spline
ifail = 0
Call g10acf(method,'W',nord,xord,yord,wwt,yhat,c,ldc,rss,df,res,h,crit, &
  rho,u,tol,maxcal,wk,ifail)

!      Display results

```

```

Write (nout,99999) 'Residual sum of squares = ', rss
Write (nout,99999) 'Degrees of freedom = ', df
Write (nout,99999) 'RHO = ', rho
Write (nout,*)
Write (nout,*) '      Input data                Output results'
Write (nout,*) '      I      X      Y                YHAT      H'
Write (nout,99998)(i,xord(i),yord(i),yhat(i),h(i),i=1,nord)

99999 Format (1X,A,F10.2)
99998 Format (I4,2F8.3,6X,2F8.3)
End Program gl0acfe

```

10.2 Program Data

G10ACF Example Program Data

```

'D' 'U' 43                                :: METHOD,WEIGHT,N
5.2 4.8
8.8 4.1 10.5 5.2 10.6 5.5 10.4 5.0
1.8 3.4 12.7 3.4 15.6 4.9 5.8 5.6
1.9 3.7 2.2 3.9 4.8 4.5 7.9 4.8
5.2 4.9 0.9 3.0 11.8 4.6 7.9 4.8
11.5 5.5 10.6 4.5 8.5 5.3 11.1 4.7
12.8 6.6 11.3 5.1 1.0 3.9 14.5 5.7
11.9 5.1 8.1 5.2 13.8 3.7 15.5 4.9
9.8 4.8 11.0 4.4 12.4 5.2 11.1 5.1
5.1 4.6 4.8 3.9 4.2 5.1 6.9 5.1
13.2 6.0 9.9 4.9 12.5 4.1 13.2 4.6
8.9 4.9 10.8 5.1                                :: End of X,Y
10000 0.001 40 12.0                             :: U,TOL,MAXCAL,CRIT

```

10.3 Program Results

G10ACF Example Program Results

```

Residual sum of squares =      10.35
Degrees of freedom =      25.00
RHO =      2.68

```

Input data			Output results	
I	X	Y	YHAT	H
1	0.900	3.000	3.373	0.534
2	1.000	3.900	3.406	0.427
3	1.800	3.400	3.642	0.313
4	1.900	3.700	3.686	0.313
5	2.200	3.900	3.839	0.448
6	4.200	5.100	4.614	0.564
7	4.800	4.200	4.576	0.442
8	5.100	4.600	4.715	0.189
9	5.200	4.850	4.783	0.407
10	5.800	5.600	5.193	0.455
11	6.900	5.100	5.184	0.592
12	7.900	4.800	4.958	0.530
13	8.100	5.200	4.931	0.234
14	8.500	5.300	4.845	0.245
15	8.800	4.100	4.763	0.271
16	8.900	4.900	4.748	0.292
17	9.800	4.800	4.850	0.301
18	9.900	4.900	4.875	0.276
19	10.400	5.000	4.970	0.173
20	10.500	5.200	4.977	0.154
21	10.600	5.000	4.979	0.285
22	10.800	5.100	4.970	0.136
23	11.000	4.400	4.961	0.137
24	11.100	4.900	4.964	0.284
25	11.300	5.100	4.975	0.162
26	11.500	5.500	4.975	0.186
27	11.800	4.600	4.930	0.213
28	11.900	5.100	4.911	0.220
29	12.400	5.200	4.852	0.206
30	12.500	4.100	4.857	0.196

31	12.700	3.400	4.900	0.189
32	12.800	6.600	4.932	0.193
33	13.200	5.300	4.955	0.488
34	13.800	3.700	4.797	0.408
35	14.500	5.700	5.076	0.559
36	15.500	4.900	4.979	0.445
37	15.600	4.900	4.946	0.535
