

NAG Fortran Library Routine Document

G02ECF

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

G02ECF calculates R^2 and C_p -values from the residual sums of squares for a series of linear regression models.

2 Specification

```

SUBROUTINE G02ECF(MEAN, N, SIGSQ, TSS, NMOD, NTERMS, RSS, RSQ, CP,
1                IFAIL)
  INTEGER          N, NMOD, NTERMS(NMOD), IFAIL
  real            SIGSQ, TSS, RSS(NMOD), RSQ(NMOD), CP(NMOD)
  CHARACTER*1      MEAN

```

3 Description

When selecting a linear regression model for a set of n observations a balance has to be found between the number of independent variables in the model and fit as measured by the residual sum of squares. The more variables included the smaller will be the residual sum of squares. Two statistics can help in selecting the best model.

- (a) R^2 represents the proportion of variation in the dependent variable that is explained by the independent variables.

$$R^2 = \frac{\text{Regression Sum of Squares}}{\text{Total Sum of Squares}},$$

where Total sum of squares = $TSS = \sum (y - \bar{y})^2$ (if mean is fitted, otherwise $TSS = \sum y^2$) and

Regression sum of squares = $\text{RegSS} = TSS - \text{RSS}$, where

$\text{RSS} = \text{residual sum of squares} = \sum (y - \hat{y})^2$.

The R^2 -values can be examined to find a model with a high R^2 -value but with small number of independent variables.

- (b) C_p statistic.

$$C_p = \frac{\text{RSS}}{\hat{\sigma}^2} - (n - 2p),$$

where p is the number of parameters (including the mean) in the model and $\hat{\sigma}^2$ is an estimate of the true variance of the errors. This can often be obtained from fitting the full model.

A well fitting model will have $C_p \simeq p$. C_p is often plotted against p to see which models are closest to the $C_p = p$ line.

G02ECF may be called after G02EAF which calculates the residual sums of squares for all possible linear regression models.

4 References

Draper N R and Smith H (1985) *Applied Regression Analysis* (2nd Edition) Wiley

Weisberg S (1985) *Applied Linear Regression* Wiley

5 Parameters

- 1: MEAN – CHARACTER*1 *Input*
On entry: indicates if a mean term is to be included.
 If MEAN = 'M' (Mean), a mean term, intercept, has been included in the model.
 If MEAN = 'Z' (Zero), the model passes through the origin, zero-point.
Constraint: MEAN = 'M' or 'Z'.

- 2: N – INTEGER *Input*
On entry: the number of observations used in the regression model, n .
Constraint: N must be greater than $2 \times p_{\max}$, where $p_{\max}$ is the largest number of independent variables fitted (including the mean if fitted).

- 3: SIGSQ – *real* *Input*
On entry: the best estimate of true variance of the errors, $\hat{\sigma}^2$.
Constraint: SIGSQ > 0.0.

- 4: TSS – *real* *Input*
On entry: the total sum of squares for the regression model.
Constraint: TSS > 0.0.

- 5: NMOD – INTEGER *Input*
On entry: the number of regression models.
Constraint: NMOD > 0.

- 6: NTERMS(NMOD) – INTEGER array *Input*
On entry: NTERMS(i) must contain the number of independent variables (not counting the mean) fitted to the i th model, for $i = 1, 2, \dots, \text{NMOD}$.

- 7: RSS(NMOD) – *real* array *Input*
On entry: RSS(i) must contain the residual sum of squares for the i th model.
Constraint: RSS(i) $\leq$ TSS, for $i = 1, 2, \dots, \text{NMOD}$.

- 8: RSQ(NMOD) – *real* array *Output*
On exit: RSQ(i) contains the R^2 -value for the i th model, for $i = 1, 2, \dots, \text{NMOD}$.

- 9: CP(NMOD) – *real* array *Output*
On exit: CP(i) contains the C_p -value for the i th model, for $i = 1, 2, \dots, \text{NMOD}$.

- 10: IFAIL – INTEGER *Input/Output*
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 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:

$IFAIL = 1$

On entry, $NMOD < 1$,
or $SIGSQ \leq 0.0$,
or $TSS \leq 0.0$.
or $MEAN \neq 'M'$ or $'Z'$.

$IFAIL = 2$

On entry, the number of parameters for a model is too large for the number of observations, i.e., $2 \times p \geq n$.

$IFAIL = 3$

On entry, $RSS(i) > TSS$, for some $i = 1, 2, \dots, NMOD$.

$IFAIL = 4$

A value of C_p is less than 0.0. This may occur if $SIGSQ$ is too large or if RSS , N or IP are incorrect.

7 Accuracy

Accuracy is sufficient for all practical purposes.

8 Further Comments

None.

9 Example

The data, from an oxygen uptake experiment, is given by Weisberg (1985). The independent and dependent variables are read and the residual sums of squares for all possible models computed using $G02EAF$. The values of R^2 and C_p are then computed and printed along with the names of variables in the models.

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.

```
*      G02ECF Example Program Text
*      Mark 14 Release.  NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          NMAX, MMAX, LMAX
      PARAMETER        (NMAX=20,MMAX=6,LMAX=32)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      real             SIGSQ, TSS
      INTEGER          I, IFAIL, II, J, M, N, NMOD
*      .. Local Arrays ..
      real             CP(LMAX), RSQ(LMAX), RSS(LMAX),
+                    WK(NMAX*(MMAX+1)), WT(NMAX), X(NMAX,MMAX),
+                    Y(NMAX)
      INTEGER          ISX(MMAX), MRANK(LMAX), NTERMS(LMAX)
```

```

      CHARACTER*3      MODEL(LMAX,MMAX), NAME(MMAX)
*      .. External Subroutines ..
      EXTERNAL         G02EAF, G02ECF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'G02ECF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, M
      IF (M.LE.MMAX .AND. N.LE.NMAX) THEN
        DO 20 I = 1, N
          READ (NIN,*) (X(I,J),J=1,M), Y(I)
20      CONTINUE
          READ (NIN,*) (ISX(J),J=1,M)
          READ (NIN,*) (NAME(J),J=1,M)
          IFAIL = 0
*
*      Calculate residual sums of squares using G02EAF
      CALL G02EAF('M','U',N,M,X,NMAX,NAME,ISX,Y,WT,NMOD,MODEL,LMAX,
+             RSS,NTERMS,MRANK,WK,IFAIL)
*
      TSS = RSS(1)
      SIGSQ = RSS(NMOD)/(N-NTERMS(NMOD)-1)
      IFAIL = 0
*
      CALL G02ECF('M',N,SIGSQ,TSS,NMOD,NTERMS,RSS,RSQ,CP,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Number of      CP      RSQ      MODEL'
      WRITE (NOUT,*) 'parameters'
      WRITE (NOUT,*)
      DO 40 I = 1, NMOD
        II = NTERMS(I)
        WRITE (NOUT,99999) II, CP(I), RSQ(I), (MODEL(I,J),J=1,II)
40      CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,I7,F11.2,F8.4,1X,5(1X,A))
      END

```

9.2 Program Data

G02ECF Example Program Data

```

20 6
 0. 1125.0 232.0 7160.0 85.9 8905.0 1.5563
 7.  920.0 268.0 8804.0 86.5 7388.0 0.8976
15.  835.0 271.0 8108.0 85.2 5348.0 0.7482
22. 1000.0 237.0 6370.0 83.8 8056.0 0.7160
29. 1150.0 192.0 6441.0 82.1 6960.0 0.3010
37.  990.0 202.0 5154.0 79.2 5690.0 0.3617
44.  840.0 184.0 5896.0 81.2 6932.0 0.1139
58.  650.0 200.0 5336.0 80.6 5400.0 0.1139
65.  640.0 180.0 5041.0 78.4 3177.0 -0.2218
72.  583.0 165.0 5012.0 79.3 4461.0 -0.1549
80.  570.0 151.0 4825.0 78.7 3901.0 0.0000
86.  570.0 171.0 4391.0 78.0 5002.0 0.0000
93.  510.0 243.0 4320.0 72.3 4665.0 -0.0969
100. 555.0 147.0 3709.0 74.9 4642.0 -0.2218
107. 460.0 286.0 3969.0 74.4 4840.0 -0.3979
122. 275.0 198.0 3558.0 72.5 4479.0 -0.1549
129. 510.0 196.0 4361.0 57.7 4200.0 -0.2218
151. 165.0 210.0 3301.0 71.8 3410.0 -0.3979
171. 244.0 327.0 2964.0 72.5 3360.0 -0.5229
220.  79.0 334.0 2777.0 71.9 2599.0 -0.0458
 0    1    1    1    1    1
'DAY' 'BOD' 'TKN' 'TS' 'TVS' 'COD'

```

9.3 Program Results

G02ECF Example Program Results

Number of parameters	CP	RSQ	MODEL			
0	55.45	0.0000				
1	56.84	0.0082	TKN			
1	20.33	0.5054	TVS			
1	13.50	0.5983	BOD			
1	6.57	0.6926	COD			
1	6.29	0.6965	TS			
2	21.36	0.5185	TKN	TVS		
2	11.33	0.6551	BOD	TVS		
2	9.09	0.6856	BOD	TKN		
2	7.70	0.7045	BOD	COD		
2	7.33	0.7095	TKN	TS		
2	7.16	0.7119	TS	TVS		
2	6.88	0.7157	BOD	TS		
2	6.87	0.7158	TKN	COD		
2	5.27	0.7376	TVS	COD		
2	1.74	0.7857	TS	COD		
3	8.68	0.7184	BOD	TKN	TVS	
3	8.16	0.7255	TKN	TS	TVS	
3	8.15	0.7256	BOD	TS	TVS	
3	7.15	0.7392	BOD	TVS	COD	
3	6.51	0.7479	BOD	TKN	COD	
3	6.25	0.7515	BOD	TKN	TS	
3	5.67	0.7595	TKN	TVS	COD	
3	3.44	0.7898	BOD	TS	COD	
3	3.42	0.7900	TS	TVS	COD	
3	2.32	0.8050	TKN	TS	COD	
4	7.70	0.7591	BOD	TKN	TS	TVS
4	6.78	0.7716	BOD	TKN	TVS	COD
4	5.07	0.7948	BOD	TS	TVS	COD
4	4.32	0.8050	BOD	TKN	TS	COD
4	4.00	0.8094	TKN	TS	TVS	COD
5	6.00	0.8094	BOD	TKN	TS	TVS COD
