

G02ECF – NAG Fortran Library Routine Document

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 , this 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 = RegSS = TSS – RSS where

RSS = 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

- [1] Draper N R and Smith H (1985) *Applied Regression Analysis* Wiley (2nd Edition)
- [2] 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. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.
On exit: IFAIL = 0 unless the routine detects an error (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 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 [2]. 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         GO2EAF, GO2ECF
*
.. 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 GO2EAF
  CALL GO2EAF('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 GO2ECF('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
