NAG Fortran Library Routine Document

G02GNF

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

G02GNF gives the estimate of an estimable function along with its standard error from the results from fitting a generalized linear model.

2 Specification

```
SUBROUTINE GO2GNF(IP, IRANK, B, COV, V, LDV, F, EST, STAT, SESTAT, Z,

TOL, WK, IFAIL)

INTEGER

IP, IRANK, LDV, IFAIL

B(IP), COV((IP*(IP+1)/2)), V(LDV,IP+7), F(IP), STAT,

SESTAT, Z, TOL, WK(IP)

LOGICAL

EST
```

3 Description

This routine computes the estimates of an estimable function for a generalized linear model which is not of full rank. It is intended for use after a call to G02GAF, G02GBF, G02GCF or G02GDF. An estimable function is a linear combination of the parameters such that it has a unique estimate. For a full rank model all linear combinations of parameters are estimable.

In the case of a model not of full rank the routines use a singular value decomposition (SVD) to find the parameter estimates, $\hat{\beta}$, and their variance-covariance matrix. Given the upper triangular matrix R obtained from the QR decomposition of the independent variables the SVD gives

$$R = Q_* \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} P^T,$$

where D is a k by k diagonal matrix with non-zero diagonal elements, k being the rank of R, and Q_* and P are p by p orthogonal matrices. This leads to a solution:

$$\hat{\beta} = P_1 D^{-1} Q_{*_1}^T c_1,$$

 P_1 being the first k columns of P, i.e., $P=(P_1P_0)$; Q_{*_1} being the first k columns of Q_* , and c_1 being the first p elements of p.

Details of the SVD are made available in the form of the matrix P^* :

$$P^* = \begin{pmatrix} D^{-1}P_1^T \\ P_0^T \end{pmatrix}$$

as described by G02GAF, G02GBF, G02GCF and G02GDF.

A linear function of the parameters, $F = f^T \beta$, can be tested to see if it is estimable by computing $\zeta = P_0^T f$. If ζ is zero, then the function is estimable, if not; the function is not estimable. In practice $|\zeta|$ is tested against some small quantity η .

Given that F is estimable it can be estimated by $f^T \hat{\beta}$ and its standard error calculated from the variance-covariance matrix of $\hat{\beta}$, C_{β} , as

$$\operatorname{se}(F) = \sqrt{f^T C_{\beta} f}.$$

[NP3546/20A] G02GNF.1

Also a z statistic

$$z = \frac{f^T \hat{\beta}}{\operatorname{se}(F)},$$

can be computed. The distribution of z will be approximately Normal.

4 References

Golub G H and van Loan C F (1996) Matrix Computations (3rd Edition) Johns Hopkins University Press, Baltimore

McCullagh P and Nelder J A (1983) Generalized Linear Models Chapman and Hall

Searle S R (1971) Linear Models Wiley

5 Parameters

1: IP – INTEGER Input

On entry: the number of terms in the linear model, p.

Constraint: $IP \geq 1$.

2: IRANK – INTEGER

On entry: the rank of the dependent variables, k.

Constraint: $1 \leq IRANK \leq IP$.

3: B(IP) - real array Input

On entry: the IP values of the estimates of the parameters of the model, $\hat{\beta}$.

4: COV((IP*(IP+1)/2)) - real array

Input

Input

On entry: the upper triangular part of the variance-covariance matrix of the IP parameter estimates given in B. They are stored packed by column, i.e., the covariance between the parameter estimate given in B(i) and the parameter estimate given in B(j), $j \ge i$, is stored in $COV(j \times (j-1)/2 + i)$.

5: V(LDV,IP+7) - real array

Input

On entry: V as returned by G02GAF, G02GBF, G02GCF and G02GDF.

6: LDV – INTEGER Input

On entry: the first dimension of the array V as declared in the (sub)program from which G02GNF is called.

Constraint: LDV \geq IP.

7: F(IP) - real array

Input

On entry: the linear function to be estimated, f.

8: EST – LOGICAL Output

On exit: EST indicates if the function was estimable.

If EST = .TRUE., then the function is estimable.

If EST = .FALSE., then the function is not estimable and STAT, SESTAT and Z are not set.

9: STAT – real Output

On exit: if EST = .TRUE., STAT contains the estimate of the function, $f^T \hat{\beta}$

G02GNF.2 [NP3546/20A]

10: SESTAT – real Output

On exit: if EST = .TRUE., SESTAT contains the standard error of the estimate of the function, se(F).

11: Z – real Output

On exit: if EST = .TRUE., Z contains the z statistic for the test of the function being equal to zero.

12: TOL – real Input

On entry: the tolerance value used in the check for estimability, η .

If TOL < 0.0, then $\sqrt{\epsilon}$, where ϵ is the *machine precision*, is used instead.

13: WK(IP) - real array

Workspace

14: 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, because for this routine the values of the output parameters may be useful even if IFAIL $\neq 0$ on exit, the recommended value is -1. 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, IP < 1, or IRANK < 1, or IRANK > IP, or LDV < IP.
```

IFAIL = 2

On entry, IRANK = IP. In this case EST is returned as true and all statistics are calculated.

IFAIL = 3

Standard error of statistic = 0.0; this may be due to rounding errors if the standard error is very small or due to mis-specified inputs COV and F.

7 Accuracy

The computations are believed to be stable.

8 Further Comments

The value of estimable functions is independent of the solution chosen from the many possible solutions. While G02GNF may be used to estimate functions of the parameters of the model as computed by G02GKF, β_c , these must be expressed in terms of the original parameters, β . The relation between the two sets of parameters may not be straightforward.

[NP3546/20A] G02GNF.3

9 Example

A loglinear model is fitted to a 3 by 5 contingency table by G02GCF. The model consists of terms for rows and columns. The table is:

```
141 67 114 79 39
131 66 143 72 35
36 14 38 28 16
```

The number of functions to be tested is read in, then the linear functions themselves are read in and tested with G02GNF. The results of G02GNF are printed.

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.

```
GO2GNF Example Program Text
   Mark 14 Release. NAG Copyright 1989.
   .. Parameters ..
   INTEGER
                     NMAX, MMAX
  PARAMETER
                     (NMAX=15, MMAX=9)
   INTEGER
                     NIN, NOUT
   PARAMETER
                     (NIN=5, NOUT=6)
   .. Local Scalars ..
   real
                     A, DEV, EPS, SESTAT, STAT, TOL, Z
  INTEGER
                     I, IDF, IFAIL, IP, IPRINT, IRANK, J, M, MAXIT, N,
                     NESTFN
  LOGICAL
                     EST
   .. Local Arrays ..
                     B(MMAX), COV((MMAX*MMAX+MMAX)/2), F(MMAX),
                     SE(MMAX), V(NMAX,7+MMAX),
                     WK((MMAX*MMAX+3*MMAX+22)/2), WT(NMAX),
                     X(NMAX,MMAX), Y(NMAX)
   INTEGER
                    ISX(MMAX)
   .. External Subroutines .
  EXTERNAL
                    GO2GCF, GO2GNF
   .. Executable Statements .
   WRITE (NOUT,*) 'G02GNF Example Program Results'
   Skip heading in data file
   READ (NIN, *)
  READ (NIN,*) N, M, IPRINT
   IF (N.LE.NMAX .AND. M.LT.MMAX) 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), IP
      Set control parameters
      EPS = 0.000001e0
      TOL = 0.00005e0
      MAXIT = 10
      IFAIL = -1
      Fit Log-linear model using G02GCF
CALL G02GCF('L','M','N','U',N,X,NMAX,M,ISX,IP,Y,WT,A,DEV,IDF,B,
                   IRANK,SE,COV,V,NMAX,TOL,MAXIT,IPRINT,EPS,WK,IFAIL)
      IF (IFAIL.EQ.O .OR. IFAIL.GE.7) THEN
         WRITE (NOUT, *)
         WRITE (NOUT, 99999) 'Deviance = ', DEV
         WRITE (NOUT, 99998) 'Degrees of freedom = ', IDF
         WRITE (NOUT, *)
         WRITE (NOUT, *)
                                Estimate
                                              Standard error'
         WRITE (NOUT, *)
         DO 40 I = 1, IP
            WRITE (NOUT, 99997) B(I), SE(I)
40
         CONTINUE
         READ (NIN, *) NESTFN
         DO 60 I = 1, NESTFN
```

G02GNF.4 [NP3546/20A]

```
READ (NIN,*) (F(J),J=1,IP)
                IFAIL = -1
                CALL GO2GNF(IP, IRANK, B, COV, V, NMAX, F, EST, STAT, SESTAT, Z,
                            TOL, WK, IFAIL)
                IF (IFAIL.EQ.O .OR. IFAIL.EQ.2) THEN
                   WRITE (NOUT, *)
                   WRITE (NOUT, 99996) 'Function', I
                   WRITE (NOUT, 99995) (F(J), J=1, IP)
                   WRITE (NOUT, *)
                   IF (EST) THEN
                      WRITE (NOUT, 99994) 'STAT = ', STAT, ' SE = ',
                        SESTAT, ' Z = ', Z
                      WRITE (NOUT,*) 'Function not estimable'
                   END IF
                END IF
   60
            CONTINUE
         END IF
      END IF
      STOP
99999 FORMAT (1X,A,e12.4)
99998 FORMAT (1X,A,I2)
99997 FORMAT (1X,2F14.4)
99996 FORMAT (1X,A,I4)
99995 FORMAT (1X,5F8.2)
99994 FORMAT (1X,A,F10.4,A,F10.4,A,F10.4)
      END
```

9.2 Program Data

```
GO2GNF Example Program Data
15 8 0
1.0 0.0 0.0 1.0 0.0 0.0 0.0 0.0 141.
1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 67.
1.0 0.0 0.0 0.0 0.0 1.0 0.0 0.0 114.
1.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0
1.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0
0.0 1.0 0.0 1.0 0.0 0.0 0.0 0.0 131.
0.0 1.0 0.0 0.0 1.0 0.0 0.0 0.0
0.0 1.0 0.0 0.0 0.0 1.0 0.0 0.0 143.
0.0 1.0 0.0 0.0 0.0 0.0 1.0 0.0
0.0 1.0 0.0 0.0 0.0 0.0 0.0 1.0
0.0 0.0 1.0 1.0 0.0 0.0 0.0 0.0
                                 36.
0.0 0.0 1.0 0.0 1.0 0.0 0.0 0.0
0.0 0.0 1.0 0.0 0.0 1.0 0.0 0.0
0.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0
0.0 0.0 1.0 0.0 0.0 0.0 0.0 1.0
                                16.
 1
        1
            1
                1
                    1
                        1
 3
 1.0 1.0 0.0 0.0 1.0 0.0 0.0 0.0 0.0
 0.0 1.0 -1.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
```

9.3 Program Results

```
GO2GNF Example Program Results
Deviance =
            0.9038E+01
Degrees of freedom = 8
      Estimate
                   Standard error
        2.5977
                      0.0258
                      0.0438
        1.2619
        1.2777
                      0.0436
        0.0580
                      0.0668
        1.0307
                      0.0551
```

[NP3546/20A] G02GNF.5

G02GNF.6 (last) [NP3546/20A]