nag_regsn_mult_linear_add_var (g02dec)

1. Purpose

nag_regsn_mult_linear_add_var (g02dec) adds a new independent variable to a general linear regression model.

2. Specification

3. Description

A linear regression model may be built up by adding new independent variables to an existing model. nag_regsn_mult_linear_add_var updates the QR decomposition used in the computation of the linear regression model. The QR decomposition may come from nag_regsn_mult_linear (g02dac) or a previous call to nag_regsn_mult_linear_add_var. The general linear regression model is defined by:

$$y = X\beta + \varepsilon$$

where y is a vector of n observations on the dependent variable, X is an n by p matrix of the independent variables of column rank k, β is a vector of length p of unknown parameters, and ε is a vector of length n of unknown random errors such that var $\varepsilon = V\sigma^2$, where V is a known diagonal matrix.

If V = I, the identity matrix, then least-squares estimation is used. If $V \neq I$, then for a given weight matrix $W \propto V^{-1}$, weighted least-squares estimation is used.

The least-squares estimates, $\hat{\beta}$ of the parameters β minimize $(y - X\beta)^T (y - X\beta)$ while the weighted least-squares estimates minimize $(y - X\beta)^T W (y - X\beta)$.

The parameter estimates may be found by computing a QR decomposition of X (or $W^{\frac{1}{2}}X$ in the weighted case), i.e.,

$$X = QR^* \quad (\text{or } W^{\frac{1}{2}}X = QR^*)$$

where $R^* = \begin{pmatrix} R \\ 0 \end{pmatrix}$ and R is a p by p upper triangular matrix and Q is an n by n orthogonal matrix.

If R is of full rank, then
$$\hat{\beta}$$
 is the solution to:

$$R\hat{\beta} = c_1$$

where $c = Q^T y$ (or $Q^T W^{\frac{1}{2}} y$) and c_1 is the first p elements of c.

If R is not of full rank a solution is obtained by means of a singular value decomposition (SVD) of R.

To add a new independent variable, x_{p+1} , R and c have to be updated. The matrix Q_{p+1} is found such that $Q_{p+1}^T[R:Q^Tx_{p+1}]$ (or $Q_{p+1}^T[R:Q^TW^{\frac{1}{2}}x_{p+1}]$) is upper triangular. The vector c is then updated by multiplying by Q_{p+1}^T .

The new independent variable is tested to see if it is linearly related to the existing independent variables by checking that at least one of the values $(Q^T x_{p+1})_i$, for $i = p+2, p+3, \ldots, n$ is non-zero.

The new parameter estimates, $\hat{\beta}$, can then be obtained by a call to nag_regsn_mult_linear_upd_model (g02ddc).

The function can be used with p = 0, in which case R and c are initialized.

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4. Parameters

 \mathbf{n}

Input: the number of observations, n.

Constraint: $\mathbf{n} \geq 1$.

ip

Input: the number of independent variables already in the model, p.

Constraint: ip > 0 and ip < n.

q[n][tdq]

Input: if $\mathbf{ip} \neq 0$, then \mathbf{q} must contain the results of the QR decomposition for the model with p parameters as returned by nag_regsn_mult_linear (g02dac) or a previous call to nag_regsn_mult_linear_add_var.

If $\mathbf{ip} = 0$, then the first column of \mathbf{q} should contain the *n* values of the dependent variable, *y*. Output: the results of the QR decomposition for the model with p + 1 parameters:

the first column of \mathbf{q} contains the updated value of c,

the columns 2 to ip + 1 are unchanged,

the first $\mathbf{ip} + 1$ elements of column $\mathbf{ip} + 2$ contain the new column of R, while the remaining $\mathbf{n} - \mathbf{ip} - 1$ elements contain details of the matrix Q_{p+1} .

tdq

Input: tdq the last dimension of the array q as declared in the function from which nag_regsn_mult_linear_add_var is called.

Constraint: $\mathbf{tdq} \geq \mathbf{ip} + 2$.

p[ip+1]

Input: \mathbf{p} contains further details of the QR decomposition used. The first \mathbf{ip} elements of \mathbf{p} must contain the zeta values for the QR decomposition (see nag_real_qr (f01qcc) for details). The first \mathbf{ip} elements of array \mathbf{p} are provided by nag_regsn_mult_linear (g02dac) or by previous calls to nag_regsn_mult_linear_add_var.

Output: the first **ip** elements of **p** are unchanged and the (**ip**+1)th element contains the zeta value for Q_{p+1} .

 $\mathbf{wt}[\mathbf{n}]$

Input: if weighted estimates are required, then **wt** must contain the weights to be used in the weighted regression. Otherwise **wt** need not be defined and may be set to the null pointer **NULL**, i.e., (double *)0.

If $\mathbf{wt}[i] = 0.0$, then the *i*th observation is not included in the model, in which case the effective number of observations is the number of observations with non-zero weights.

If $\mathbf{wt} = \mathbf{NULL}$, then the effective number of observations is n.

Constraint: $\mathbf{wt} = \mathbf{NULL}$ or $\mathbf{wt}[i] \ge 0.0$, for $i = 0, 1, \dots, n-1$.

x[n]

Input: the new independent variable, x.

rss

Output: the residual sum of squares for the new fitted model.

Note: this will only be valid if the model is of full rank, see Section 6.

tol

Input: the value of tol is used to decide if the new independent variable is linearly related to independent variables already included in the model. If the new variable is linearly related then c is not updated. The smaller the value of tol the stricter the criterion for deciding if there is a linear relationship.

Suggested value: tol = 0.000001.

Constraint: tol > 0.0.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

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5. Error Indications and Warnings

NE_INT_ARG_LT

On entry, **n** must not be less than 1: $\mathbf{n} = \langle value \rangle$. On entry, **ip** must not be less than 0: $\mathbf{ip} = \langle value \rangle$.

NE_2_INT_ARG_GE

On entry $i\mathbf{p} = \langle value \rangle$ while $\mathbf{n} = \langle value \rangle$. These parameters must satisfy $i\mathbf{p} < \mathbf{n}$.

NE_2_INT_ARG_LT

On entry $\mathbf{tdq} = \langle value \rangle$ while $\mathbf{ip}+2 = \langle value \rangle$. These parameters must satisfy $\mathbf{tdq} \geq \mathbf{ip}+2$.

NE_REAL_ARG_LT

On entry, $\mathbf{wt}[\langle value \rangle]$ must not be less than 0.0: $\mathbf{wt}[\langle value \rangle] = \langle value \rangle$.

NE_REAL_ARG_LE

On entry, **tol** must not be less than or equal to 0.0: **tol** = $\langle value \rangle$.

NE_NVAR_NOT_IND

The new independent variable is a linear combination of existing variables. The $(\mathbf{ip}+1)$ th column of \mathbf{q} is, therefore, null.

6. Further Comments

It should be noted that the residual sum of squares produced by nag_regsn_mult_linear_add_var may not be correct if the model to which the new independent variable is added is not of full rank. In such a case nag_regsn_mult_linear_upd_model (g02ddc) should be used to calculate the residual sum of squares.

6.1. Accuracy

The accuracy is closely related to the accuracy of nag_real_apply_q (f01qdc) which should be consulted for further details.

6.2. References

Draper N R and Smith H (1985) Applied Regression Analysis (2nd Edn) Wiley.

Golub G H and Van Loan C F (1983) *Matrix Computations* Johns Hopkins University Press, Baltimore.

Hammarling S (1985) The Singular Value Decomposition in Multivariate Statistics *ACM Signum Newsletter* **20** (3) 2–25.

McCullagh P and Nelder J A (1983) Generalized Linear Models Chapman and Hall. Searle S R (1971) Linear Models Wiley.

7. See Also

nag_real_qr (f01qcc) nag_real_apply_q (f01qdc) nag_regsn_mult_linear (g02dac) nag_regsn_mult_linear_upd_model (g02ddc) nag_regsn_mult_linear_delete_var (g02dfc)

8. Example

A data set consisting of 12 observations is read in. The four independent variables are stored in the array \mathbf{x} while the dependent variable is read into the first column of \mathbf{q} . If the character variable **meanc** indicates that a mean should be included in the model, a variable taking the value 1.0 for all observations is set up and fitted. Subsequently, one variable at a time is selected to enter the model as indicated by the input value of \mathbf{indx} . After the variable has been added the parameter estimates are calculated by nag_regsn_mult_linear_upd_model (g02ddc) and the results printed. This is repeated until the input value of \mathbf{indx} is 0.

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8.1. Program Text

```
/* nag_resgn_mult_linear_add_var(g02dec) Example Program
 * Copyright 1991 Numerical Algorithms Group.
 * Mark 2, 1991.
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagg02.h>
#define NMAX 12
#define MMAX 5
#define TDX MMAX
#define TDQ MMAX+1
main()
{
  double rss, rsst, tol;
Integer i, indx, ip, rank, j, m, n;
  double df;
  Boolean svd;
  char meanc, weight;
  Nag_IncludeMean mean;
double b[MMAX], cov[MMAX*(MMAX+1)/2], p[MMAX*(MMAX+2)],
  q[NMAX][MMAX+1], se[MMAX], wt[NMAX], x[NMAX][MMAX], xe[NMAX];
  double
           *wtptr;
  static
            NagError fail;
  Vprintf("g02dec Example Program Results\n");
  /* Skip heading in data file */
Vscanf("%*[^\n]");
Vscanf("%ld %ld %c %c", &n, &m, &weight, &meanc);
  if (meanc=='m')
    mean = Nag_MeanInclude;
  else
    mean = Nag_MeanZero;
  if (weight=='w')
    wtptr = wt;
  else
    wtptr = (double *)0;
  if (n<=NMAX && m<MMAX)
       if (wtptr)
         {
            for (i=0; i<n; i++)
                for (j=0; j<m; j++)
  Vscanf("%lf", &x[i][j]);
Vscanf("%lf%lf", &q[i][0], &wt[i]);</pre>
         }
       else
         {
            for (i=0; i<n; i++)
                for (j=0; j<m; j++)
  Vscanf("%lf", &x[i][j]);</pre>
                 Vscanf("%lf", &q[i][0]);
         }
       /* Set tolerance */
       tol = 0.000001e0;
       ip = 0;
       if (mean==Nag_MeanInclude)
```

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```
for (i = 0; i < n; ++i)
                 xe[i] = 1.0;
               g02dec(n, ip, (double *)q, (Integer)(TDQ), p, wtptr, xe, &rss,
                       tol, NAGERR_DEFAULT);
               ip = 1;
           while(scanf("%ld", &indx)!=EOF)
             {
               if (indx>0)
                   for (i=0; i<n; i++)
                     xe[i] = x[i][indx-1];
                   if (fail.code==NE_NOERROR)
                      {
                        ip += 1;
                        Vprintf("Variable %4ld added\n", indx);
                        rsst = 0.0;
                        g02ddc(n, ip, (double *)q, (Integer)(TDQ), \&rsst, \&df, b, se,
                               cov, &svd, &rank, p, tol, NAGERR_DEFAULT);
                          Vprintf("Model not of full rank\n\n");
                        Vprintf("Residual sum of squares = %13.4e\n", rsst);
                        Vprintf("Degrees of freedom = %3.1f\n\n", df);
Vprintf("Variable Parameter estimate Standard error\n\n")
                        for (j=0; j<ip; j++)
    Vprintf("%6ld%20.4e%20.4e\n", j+1, b[j], se[j]);</pre>
                        Vprintf("\n");
                      }
                   else if (fail.code==NE_NVAR_NOT_IND)
                      Vprintf(" * New variable not added *\n");
                   else
                      {
                        Vprintf("%s\n", fail.message);
                        exit(EXIT_FAILURE);
                 }
             }
         }
       else
     Vfprintf(stderr, "One or both of m and n are out of range:\ m = \%-31d while n = \%-31d\n", m, n);
           exit(EXIT_FAILURE);
       exit(EXIT_SUCCESS);
8.2. Program Data
     g02dec Example Program Data
      12 4 u m
     1.0 1.4 0.0 0.0 4.32
     1.5 2.2 0.0 0.0 5.21
     2.0 4.5 0.0 0.0 6.49
     2.5 6.1 0.0 0.0 7.10
     3.0 7.1 0.0 0.0 7.94
     3.5 7.7 0.0 0.0 8.53
     4.0 8.3 1.0 4.0 8.84
     4.5 8.6 1.0 4.5 9.02
     5.0 8.8 1.0 5.0 9.27
     5.5 9.0 1.0 5.5 9.43
     6.0 9.3 1.0 6.0 9.68
     6.5 9.2 1.0 6.5 9.83
     1
     3
```

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8.3. Program Results

g02dec Example Program Results

Variable 1 added Residual sum of squares = 4.0164e+00

Degrees of freedom = 10.0

Variable Parameter estimate Standard error

1 4.4100e+00 4.3756e-01 2 9.4979e-01 1.0599e-01

Variable 3 added

Residual sum of squares = 3.8872e+00

Degrees of freedom = 9.0

Variable Parameter estimate Standard error

1 4.2236e+00 5.6734e-01 2 1.0554e+00 2.2217e-01 3 -4.1962e-01 7.6695e-01

Variable 4 added

Residual sum of squares = 1.8702e-01

Degrees of freedom = 8.0

Variable Parameter estimate Standard error

1 2.7605e+00 1.7592e-01 2 1.7057e+00 7.3100e-02 3 4.4575e+00 4.2676e-01 4 -1.3006e+00 1.0338e-01

Variable 2 added

Residual sum of squares = 8.4066e-02

Degrees of freedom = 7.0

Variable Parameter estimate Standard error 1.8181e-01 1 3.1440e+00 2 9.0748e-01 2.7761e-01 3 8.6804e-01 2.0790e+00 2.4530e-01 4 -6.1589e-01 5 2.9224e-01 9.9810e-02

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