

## 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

```
#include <nag.h>
#include <nagg02.h>

void nag_regsn_mult_linear_add_var(Integer n, Integer ip, double q[],
    Integer tdq, double p[], double wt[], double x[], double *rss,
    double tol, NagError *fail)
```

### 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  $k$ ,  $\beta$  is a vector of length  $p$  of unknown parameters, and  $\varepsilon$  is a vector of length  $n$  of unknown random errors such that  $\text{var } \varepsilon = V\sigma^2$ , 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  $\beta$  minimize  $(y - X\beta)^T(y - X\beta)$  while the weighted least-squares estimates minimize  $(y - X\beta)^TW(y - X\beta)$ .

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  $Q_{p+1}^T[R : Q^T x_{p+1}]$  (or  $Q_{p+1}^T[R : Q^T W^{\frac{1}{2}} x_{p+1}]$ ) 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  $i = p+2, p+3, \dots, n$  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.

## 4. Parameters

**n**

Input: the number of observations,  $n$ .  
 Constraint:  $n \geq 1$ .

**ip**

Input: the number of independent variables already in the model,  $p$ .  
 Constraint:  $ip \geq 0$  and  $ip < n$ .

**q[n][tdq]**

Input: if  $ip \neq 0$ , then **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  $ip = 0$ , then the first column of **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 **q** contains the updated value of  $c$ ,

the columns 2 to  $ip + 1$  are unchanged,

the first  $ip + 1$  elements of column  $ip + 2$  contain the new column of  $R$ , while the remaining  $n - ip - 1$  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:  $tdq \geq ip + 2$ .

**p[ip+1]**

Input: **p** contains further details of the  $QR$  decomposition used. The first  $ip$  elements of **p** must contain the zeta values for the  $QR$  decomposition (see nag\_real\_qr (f01qcc) for details).

The first  $ip$  elements of array **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  $Q_{p+1}$ .

**wt[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  $wt[i] = 0.0$ , 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 **wt** = **NULL**, then the effective number of observations is  $n$ .

Constraint: **wt** = **NULL** or  $wt[i] \geq 0.0$ , 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.

## 5. Error Indications and Warnings

### NE\_INT\_ARG\_LT

On entry, **n** must not be less than 1: **n** =  $\langle value \rangle$ .

On entry, **ip** must not be less than 0: **ip** =  $\langle value \rangle$ .

### NE\_2\_INT\_ARG\_GE

On entry **ip** =  $\langle value \rangle$  while **n** =  $\langle value \rangle$ . These parameters must satisfy **ip** < **n**.

### NE\_2\_INT\_ARG\_LT

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

### NE\_REAL\_ARG\_LT

On entry, **wt**[ $\langle value \rangle$ ] must not be less than 0.0: **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 (**ip**+1)th column of **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 **x** while the dependent variable is read into the first column of **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 **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 **indx** is 0.

## 8.1. Program Text

```

/* nag_regsn_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]);
            }
        }
        else
        {
            for (i=0; i<n; i++)
            {
                for (j=0; j<m; j++)
                    Vscanf("%lf", &x[i][j]);
                Vscanf("%lf", &q[i][0]);
            }
        }
        /* Set tolerance */
        tol = 0.000001e0;
        ip = 0;
        if (mean==Nag_MeanInclude)
        {

```

```

    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];
        g02dec(n, ip, (double *)q, (Integer)(TDQ), p, wtptr, xe, &rss,
              tol, &fail);
        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);

            if (svd)
                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]);
            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:\n
m = %-3ld while n = %-3ld\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

```

4  
2  
0

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	3.1440e+00	1.8181e-01
2	9.0748e-01	2.7761e-01
3	2.0790e+00	8.6804e-01
4	-6.1589e-01	2.4530e-01
5	2.9224e-01	9.9810e-02