

# NAG C Library Function Document

## nag\_ml\_mixed\_regsn (g02jbc)

### 1 Purpose

nag\_ml\_mixed\_regsn (g02jbc) fits a linear mixed effects regression model using maximum likelihood (ML).

### 2 Specification

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

void nag_ml_mixed_regsn (Integer n, Integer ncol, const double dat[],
    Integer tddat, const Integer levels[], Integer yvid, Integer cwid, Integer nfv,
    const Integer fvid[], Integer fint, Integer nrv, const Integer rvid[],
    Integer nvpr, const Integer vpr[], Integer rint, Integer svid, double gamma[],
    Integer *nff, Integer *nrf, Integer *df, double *ml, Integer lb, double b[],
    double se[], Integer maxit, double tol, Integer *warn, NagError *fail)
```

### 3 Description

nag\_ml\_mixed\_regsn (g02jbc) fits a model of the form:

$$y = X\beta + Z\nu + \epsilon$$

where  $y$  is a vector of  $n$  observations on the dependent variable,

$X$  is a known  $n$  by  $p$  design matrix for the fixed independent variables,

$\beta$  is a vector of length  $p$  of unknown *fixed effects*,

$Z$  is a known  $n$  by  $q$  design matrix for the random independent variables,

$\nu$  is a vector of length  $q$  of unknown *random effects*;

and  $\epsilon$  is a vector of length  $n$  of unknown random errors.

Both  $\nu$  and  $\epsilon$  are assumed to have a Gaussian distribution with expectation zero and

$$\text{Var} \begin{bmatrix} \nu \\ \epsilon \end{bmatrix} = \begin{bmatrix} G & 0 \\ 0 & R \end{bmatrix}$$

where  $R = \sigma_R^2 I$ ,  $I$  is the  $n \times n$  identity matrix and  $G$  is a diagonal matrix. It is assumed that the random variables,  $Z$ , can be subdivided into  $g \leq q$  groups with each group being identically distributed with expectations zero and variance  $\sigma_i^2$ . The diagonal elements of matrix  $G$  therefore take one of the values  $\{\sigma_i^2 : i = 1, \dots, g\}$ , depending on which group the associated random variable belongs to.

The model therefore contains three sets of unknowns, the fixed effects,  $\beta$ , the random effects  $\mu$  and a vector of  $g + 1$  variance components,  $\gamma$ , where  $\gamma = \{\sigma_1^2, \sigma_2^2, \dots, \sigma_{g-1}^2, \sigma_g^2, \sigma_R^2\}$ . Rather than working directly with  $\gamma$ , nag\_ml\_mixed\_regsn (g02jbc) uses an iterative process to estimate  $\gamma^* = \{\sigma_1^2/\sigma_R^2, \sigma_2^2/\sigma_R^2, \dots, \sigma_{g-1}^2/\sigma_R^2, \sigma_g^2/\sigma_R^2, 1\}$ . Due to the iterative nature of the estimation a set of initial values,  $\gamma_0$ , for  $\gamma^*$  is required. nag\_ml\_mixed\_regsn (g02jbc) allows these initial values either to be supplied by you or calculated from the data using the minimum variance quadratic unbiased estimators (MIVQUE0) suggested by Rao (1972).

nag\_ml\_mixed\_regsn (g02jbc) fits the model using a quasi-Newton algorithm to maximize the log-likelihood function:

$$-2l_R = \log(|V|) + (n) \log(r'V^{-1}r) + \log(2\pi/n)$$

where

$$V = ZGZ' + R, \quad r = y - Xb \quad \text{and} \quad b = (X'V^{-1}X)^{-1}X'V^{-1}y.$$

Once the final estimates for  $\gamma^*$  have been obtained, the value of  $\sigma_R^2$  is given by:

$$\sigma_R^2 = (r'V^{-1}r)/(n - p).$$

Case weights,  $W_c$ , can be incorporated into the model by replacing  $X'X$  and  $Z'Z$  with  $X'W_cX$  and  $Z'W_cZ$  respectively, for a diagonal weight matrix  $W_c$ .

The log-likelihood,  $l_R$ , is calculated using the sweep algorithm detailed in Wolfinger *et al.* (1994).

## 4 References

- Goodnight J H (1979) A Tutorial on the SWEEP operator *The American Statistician* **33** (3) 149–158
- Harville D A (1977) Maximum likelihood approaches to variance component estimation and to related problems *JASA* **72** 320–340
- Rao C R (1972) Estimation of variance and covariance components in a linear model *J. Am. Stat. Assoc.* **67** 112–115
- Stroup W W (1989) Predictable functions and prediction space in the mixed model procedure *Applications of Mixed Models in Agriculture and Related Disciplines Southern Cooperative Series Bulletin No. 343* 39–48
- Wolfinger R, Tobias R and Sall J (1994) Computing Gaussian Likelihoods and Their Derivatives for General Linear Mixed Models *SIAM Sci. Statist. Comput.* **15** 1294–1310

## 5 Arguments

- 1: **n** – Integer *Input*  
*On entry:*  $n$ , the number of observations.  
*Constraint:*  $n \geq 1$ .
- 2: **ncol** – Integer *Input*  
*On entry:* the number of columns in the data matrix, **dat**.  
*Constraint:*  $ncol \geq 2$ .
- 3: **dat**[**tddat** × **n**] – const double *Input*  
**Note:** where **DAT**( $i, j$ ) appears in this document, it refers to the array element **dat**[( $i - 1$ ) × **tddat** +  $j - 1$ ].  
*On entry:* array containing all of the data. For the  $i$ th observation:  
**DAT**( $i, yvid$ ) holds the dependent variable,  $y$ .  
If **cwid**  $\neq 0$  then **DAT**( $i, cwid$ ) holds the case weights.  
If **svid**  $\neq 0$  then **DAT**( $i, svid$ ) holds the subject variable.  
The remaining columns hold the values of the independent variables.  
*Constraints:*  
if **cwid**  $\neq 0$ , **DAT**( $i, cwid$ )  $\geq 0$ ;  
if **levels**[ $j - 1$ ]  $\neq 1$ , **DAT**( $i, j$ )  $> 0$ , **DAT**( $i, j$ )  $\leq$  **levels**[ $j - 1$ ].
- 4: **tddat** – Integer *Input*  
*On entry:* the stride separating column elements in the array **dat**.  
*Constraint:* **tddat**  $\geq n$

- 5: **levels[ncol]** – const Integer *Input*  
*On entry:* **levels**[ $i - 1$ ] contains the number of levels associated with the  $i$ th variable of the data matrix **DAT**. If this variable is continuous or binary (i.e., only takes the values zero or one) then **levels**[ $i - 1$ ] should be 1; if the variable is discrete then **levels**[ $i - 1$ ] is the number of levels associated with it and **DAT**( $j, i$ ) is assumed to take the values 1 to **levels**[ $i - 1$ ], for  $j = 1, 2, \dots, n$ .  
*Constraint:* **levels**[ $i - 1$ ]  $\geq 1$ , for  $i = 1, 2, \dots, \mathbf{ncol}$ .
- 6: **yvid** – Integer *Input*  
*On entry:* the column of **DAT** holding the dependent,  $y$ , variable.  
*Constraint:*  $1 \leq \mathbf{yvid} \leq \mathbf{ncol}$ .
- 7: **cwid** – Integer *Input*  
*On entry:* the column of **DAT** holding the case weights. If **cwid** = 0 then no weights are used.  
*Constraint:*  $0 \leq \mathbf{cwid} \leq \mathbf{ncol}$ .
- 8: **nfv** – Integer *Input*  
*On entry:* the number of independent variables in the model which are to be treated as being fixed.  
*Constraint:*  $0 \leq \mathbf{nfv} < \mathbf{ncol}$ .
- 9: **fvid[nfv]** – const Integer *Input*  
*On entry:* the columns of the data matrix **DAT** holding the fixed independent variables with **fvid**[ $i - 1$ ] holding the column number corresponding to the  $i$ th fixed variable.  
*Constraint:*  $1 \leq \mathbf{fvid}[i - 1] \leq \mathbf{ncol}$ , for  $i = 1, 2, \dots, \mathbf{nfv}$ .
- 10: **fint** – Integer *Input*  
*On entry:* flag indicating whether a fixed intercept is included (**fint** = 1).  
*Constraint:* **fint** = 0 or 1.
- 11: **nrv** – Integer *Input*  
*On entry:* the number of independent variables in the model which are to be treated as being random.  
*Constraint:*  $0 \leq \mathbf{nrv} < \mathbf{ncol}$ .
- 12: **rvid[nrv]** – const Integer *Input*  
*On entry:* the columns of the data matrix **DAT** holding the random independent variables with **rvid**[ $i - 1$ ] holding the column number corresponding to the  $i$ th random variable.  
*Constraint:*  $1 \leq \mathbf{rvid}[i - 1] \leq \mathbf{ncol}$ , for  $i = 1, 2, \dots, \mathbf{nrv}$ .
- 13: **nvpr** – Integer *Input*  
*On entry:* if **rint** = 1 and **svid**  $\neq 0$ , **nvpr** is the number of variance components being estimated – 2, ( $g - 1$ ), else **nvpr** =  $g$ . If **nrv** = 0, **nvpr** is not referenced.  
*Constraint:* if **nrv**  $\neq 0$ ,  $1 \leq \mathbf{nvpr} \leq \mathbf{nrv}$ .
- 14: **vpr[nrv]** – const Integer *Input*  
*On entry:* **vpr**[ $i - 1$ ] holds a flag indicating the variance of the  $i$ th random variable. The variance of the  $i$ th random variable is  $\sigma_j^2$ , where  $j = \mathbf{vpr}[i - 1] + 1$  if **rint** = 0 and **svid**  $\neq 0$  and  $j = \mathbf{vpr}[i - 1]$  otherwise. Random variables with the same value of  $j$  are assumed to be taken from the same distribution.  
*Constraint:*  $1 \leq \mathbf{vpr}[i - 1] \leq \mathbf{nvpr}$ , for  $i = 1, 2, \dots, \mathbf{nrv}$ .

- 15: **rint** – Integer *Input*  
*On entry:* flag indicating whether a random intercept is included (**rint** = 1). If **svid** = 0 **rint** is not referenced.  
*Constraint:* **rint** = 0 or 1.
- 16: **svid** – Integer *Input*  
*On entry:* the column of **DAT** holding the subject variable. If **svid** = 0 then no subject variable is used.  
 Specifying a subject variable is equivalent to specifying the interaction between that variable and all of the random-effects. Letting the notation  $Z_1 \times Z_S$  denote the interaction between variables  $Z_1$  and  $Z_S$ , fitting a model with **rint** = 0, random-effects  $Z_1 + Z_2$  and subject variable  $Z_S$  is equivalent to fitting a model with random-effects  $Z_1 \times Z_S + Z_2 \times Z_S$  and no subject variable. If **rint** = 1 the model is equivalent to fitting  $Z_S + Z_1 \times Z_S + Z_2 \times Z_S$  and no subject variable.  
*Constraint:*  $0 \leq \mathbf{svid} \leq \mathbf{ncol}$ .
- 17: **gamma**[**nvpr** + 2] – double *Input/Output*  
*On entry:* holds the initial values of the variance components,  $\gamma_0$ , with **gamma**[ $i - 1$ ] the initial value for  $\sigma_i^2 / \sigma_R^2$ ,  $i = 1, 2, \dots, g$ . If **rint** = 1 and **svid**  $\neq$  0 then  $g = \mathbf{nvpr} + 1$ , else  $g = \mathbf{nvpr}$ .  
 If **gamma**[0] = -1 then the remaining elements of **gamma** are ignored and the initial values for the variance components are estimated from the data using MIVQUE0.  
*On exit:* **gamma**[ $i - 1$ ], for  $i = 1, 2, \dots, g$  holds the final estimate of  $\sigma_i^2$  and **gamma**[ $g$ ] holds the final estimate for  $\sigma_R^2$ .  
*Constraint:* **gamma**[0] = -1 or **gamma**[ $i - 1$ ]  $\geq$  0, for  $i = 1, 2, \dots, g$ .
- 18: **nff** – Integer \* *Output*  
*On exit:* the number of fixed effects estimated (i.e., the number of columns,  $p$ , in the design matrix  $X$ ).
- 19: **nrf** – Integer \* *Output*  
*On exit:* the number of random effects estimated (i.e., the number of columns,  $q$ , in the design matrix  $Z$ ).
- 20: **df** – Integer \* *Output*  
*On exit:* the degrees of freedom.
- 21: **ml** – double \* *Output*  
*On exit:*  $-2l_R(\hat{\gamma})$  where  $l_R$  is the log of the maximum likelihood calculated at  $\hat{\gamma}$ , the estimated variance components returned in **gamma**.
- 22: **lb** – Integer *Input*  
*On entry:* the size of the array **b**.  
*Constraint:*  $\mathbf{lb} \geq \mathbf{fint} + \sum_{i=1}^{\mathbf{nfv}} \max(\mathbf{levels}[\mathbf{fvid}[i - 1]] - 1, 1) + L_S \times \left( \mathbf{rint} + \sum_{i=1}^{\mathbf{nrV}} \mathbf{levels}[\mathbf{rvid}[i - 1]] \right)$  where  $L_S = \mathbf{levels}[\mathbf{svid} - 1]$  if **svid**  $\neq$  0 and 1 otherwise

23: **b[lb]** – double

Output

*On exit:* the argument estimates,  $(\beta, \nu)$ , with the first **nff** elements of **b** containing the fixed effect argument estimates,  $\beta$  and the next **nrf** elements of **b** containing the random effect argument estimates,  $\nu$ .

**Fixed effects**

If  **fint** = 1, **b**[0] contains the estimate of the fixed intercept. Let  $L_i$  denote the number of levels associated with the  $i$ th fixed variable, that is  $L_i = \mathbf{levels}[\mathbf{fvid}[i - 1] - 1]$ . Define

if  **fint** = 1,  $F_1 = 2$  else if  **fint** = 0,  $F_1 = 1$ ;

$F_{i+1} = F_i + \max(L_i - 1, 1)$ ,  $i \geq 1$ .

Then for  $i = 1, 2, \dots, \mathbf{nfv}$ :

if  $L_i > 1$ , **b**[ $F_i + j - 3$ ] contains the argument estimate for the  $j$ th level of the  $i$ th fixed variable,  $j = 2, 3, \dots, L_i$ ;

if  $L_i \leq 1$ , **b**[ $F_i - 1$ ] contains the argument estimate for the  $i$ th fixed variable.

**Random effects**

Redefining  $L_i$  to denote the number of levels associated with the  $i$ th random variable, that is  $L_i = \mathbf{levels}[\mathbf{rvid}[i - 1] - 1]$ . Define

if  **rint** = 1,  $R_1 = 2$  else if  **rint** = 0,  $R_1 = 1$ ;

$R_{i+1} = R_i + L_i$ ,  $i \geq 1$ .

Then for  $i = 1, 2, \dots, \mathbf{nrv}$ :

if  **svid** = 0,

if  $L_i > 1$ , **b**[**nff** +  $R_i + j - 2$ ] contains the argument estimate for the  $j$ th level of the  $i$ th random variable,  $j = 1, 2, \dots, L_i$ ;

if  $L_i \leq 1$ , **b**[**nff** +  $R_i - 1$ ] contains the argument estimate for the  $i$ th random variable;

if  **svid**  $\neq$  0,

let  $L_S$  denote the number of levels associated with the subject variable, that is  $L_S = \mathbf{levels}[\mathbf{svid} - 1]$ ;

if  $L_i > 1$ , **b**[**nff** +  $(s - 1)L_S + R_i + j - 2$ ] contains the argument estimate for the interaction between the  $s$ th level of the subject variable and the  $j$ th level of the  $i$ th random variable,  $s = 1, 2, \dots, L_S$  and  $j = 1, 2, \dots, L_i$ ;

if  $L_i \leq 1$ , **b**[**nff** +  $(s - 1)L_S + R_i - 1$ ] contains the argument estimate for the interaction between the  $s$ th level of the subject variable and the  $i$ th random variable,  $s = 1, 2, \dots, L_S$ ;

if  **rint** = 1, **b**(**nff** + 1) contains the estimate of the random intercept.

24: **se[lb]** – double

Output

*On exit:* the standard errors of the argument estimates given in **b**.

25: **maxit** – Integer

Input

*On entry:* the maximum number of iterations.

**maxit** < 0

The default value of 100 is used.

**maxit** = 0

The argument estimates  $(\beta, \mu)$  and corresponding standard errors are calculated based on the value of  $\gamma_0$  supplied in **gamma**.

26: **tol** – double

Input

*On entry:* the tolerance used to assess convergence. If **tol** = 0 then the default value of  $\epsilon^{0.7}$  is used, where  $\epsilon$  is the *machine precision*.

- 27: **warn** – Integer \* *Output*  
*On exit:* is set to 1 if a variance component was estimated to be a negative value during the fitting process. Otherwise **warn** is set to 0.  
 If **warn** = 1, the negative estimate is set to zero and the estimation process allowed to continue.
- 28: **fail** – NagError \* *Input/Output*  
 The NAG error argument (see Section 2.6 of the Essential Introduction).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

### NE\_BAD\_PARAM

On entry, invalid data: categorical variable with value greater than that specified in **levels**.

### NE\_CONV

Routine failed to converge in **maxit** iterations: **maxit** =  $\langle value \rangle$ .

### NE\_FAIL\_TOL

Routine failed to converge to specified tolerance: **tol** =  $\langle value \rangle$ .

### NE\_INT

On entry, **fint**  $\neq$  0 and **fint**  $\neq$  1 : **fint** =  $\langle value \rangle$ .

On entry, **fvid**[*i*] < 1 or **fvid**[*i*] > **ncol**, for at least one *i* : **ncol** =  $\langle value \rangle$ .

On entry, **lb** too small: **lb** =  $\langle value \rangle$ .

On entry, **levels**[*i*] < 1, for at least one *i*.

On entry, **n** =  $\langle value \rangle$ .

Constraint: **n**  $\geq$  1.

On entry, **ncol** =  $\langle value \rangle$ .

Constraint: **ncol**  $\geq$  2.

On entry, **rint**  $\neq$  0 and **rint**  $\neq$  1 : **rint** =  $\langle value \rangle$ .

On entry, **rvid**[*i*] < 1 or **rvid**[*i*] > **ncol**, for at least one *i* : **ncol** =  $\langle value \rangle$ .

On entry, **tddat** =  $\langle value \rangle$ .

Constraint: **tddat** > 0.

On entry, **vpr**[*i*] < 1 or **vpr**[*i*] > **nvpr**, for at least one *i* : **nvpr** =  $\langle value \rangle$ .

### NE\_INT\_2

On entry, **cwid** < 0 or **cwid** > **ncol** or -ve weight: **cwid** =  $\langle value \rangle$ , **ncol** =  $\langle value \rangle$ .

On entry, **nfv** < 0 or **nfv**  $\geq$  **ncol**: **nfv** =  $\langle value \rangle$ , **ncol** =  $\langle value \rangle$ .

On entry, **nrsv** < 0 or **nrsv**  $\geq$  **ncol**: **nrsv** =  $\langle value \rangle$ , **ncol** =  $\langle value \rangle$ .

On entry, **nvpr** < 0 or **nvpr** > **nrsv** or (**nrsv** > 0 and **nvpr** < 1): **nvpr** =  $\langle value \rangle$ , **nrsv** =  $\langle value \rangle$ .

On entry, **svid** < 0 or **svid** > **ncol**: **svid** =  $\langle value \rangle$ , **ncol** =  $\langle value \rangle$ .

On entry, **tddat** < **n** : **tddat** =  $\langle value \rangle$ , **n** =  $\langle value \rangle$ .

On entry, **tddat** =  $\langle value \rangle$ , **n** =  $\langle value \rangle$ .

Constraint: **tddat**  $\geq$  **n**.

On entry, **yvid** < 1 or **yvid** > **ncol**: **yvid** =  $\langle value \rangle$ , **ncol** =  $\langle value \rangle$ .

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

### NE\_REAL

On entry, **gamma**[*i*] < 0, for at least one *i*.

### NE\_ZERO\_DOF\_ERROR

Degrees of freedom < 1: **df** =  $\langle value \rangle$ .

## 7 Accuracy

The accuracy of the results can be adjusted through the use of the **tol** argument.

## 8 Further Comments

Wherever possible any block structure present in the design matrix *Z* should be modelled through a subject variable, specified via **svid**, rather than being explicitly entered into **dat**.

nag\_ml\_mixed\_regsn (g02jbc) uses an iterative process to fit the specified model and for some problems this process may fail to converge (see **fail.code** = **NE\_FAIL\_TOL**). If the function fails to converge then the maximum number of iterations (see **maxit**) or tolerance (see **tol**) may require increasing. Alternatively, the model can be fit using restricted maximum likelihood (see nag\_reml\_mixed\_regsn (g02jac)) or using the non-iterative MIVQUE0.

To fit the model just using MIVQUE0, the first element of **gamma** should be set to  $-1$  and **maxit** should be set to zero.

Although the quasi-Newton algorithm used in nag\_ml\_mixed\_regsn (g02jbc) tends to require more iterations before converging compared to the Newton–Raphson algorithm recommended by Wolfinger *et al.* (1994), it does not require the second derivatives of the likelihood function to be calculated and consequentially takes significantly less time per iteration.

## 9 Example

The following dataset is taken from Stroup (1989) and arises from a balanced split-plot design with the whole plots arranged in a randomized complete block-design.

In this example the full design matrix for the random independent variable,  $Z$ , is given by:

$$Z = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} A & 0 & 0 & 0 \\ 0 & A & 0 & 0 \\ 0 & 0 & A & 0 \\ 0 & 0 & 0 & A \\ A & 0 & 0 & 0 \\ 0 & A & 0 & 0 \\ 0 & 0 & A & 0 \\ 0 & 0 & 0 & A \end{pmatrix}, \quad (1)$$

where

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

The block structure evident in (1) is modelled by specifying a four-level subject variable, taking the values  $\{1, 1, 1, 2, 2, 2, 3, 3, 3, 4, 4, 4, 1, 1, 1, 2, 2, 2, 3, 3, 3, 4, 4, 4\}$ . The first column of 1s is added to  $A$  by setting  $\mathbf{rint} = 1$ . The remaining columns of  $A$  are specified by a three level factor, taking the values,  $\{1, 2, 3, 1, 2, 3, 1, \dots\}$ .

## 9.1 Program Text

```
/* nag_ml_mixed_regsn (g02jbc) Example Program.
 *
 * Copyright 2004 Numerical Algorithms Group.
 *
 * Mark 8, 2004.
 */
```

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

```
int main(void)
```

```

{
/* Scalars */
double like, tol;
Integer cwid, df, exit_status, fint, i, j, k, l, lb, maxit, n, ncol, nff, nfv;
Integer nrf, nrv, nv, nvpr, tddat, rint, svid, warnp, yvid, fnlevel, rnlevel;
Integer lgamma, fl;
/* Nag types */
NagError fail;

/* Arrays */
double *b=0, *dat=0, *gamma=0, *se=0;
Integer *fvid=0, *levels=0, *rvid=0, *vpr=0;

#define DAT(I,J) dat[(I-1)*tddat + J - 1]

exit_status = 0;
INIT_FAIL(fail);
Vprintf("nag_ml_mixed_regsn (g02jbc) Example Program Results\n\n");
lb = 25;
/* Skip heading in data file */
Vscanf("%*[\n] ");

/* Read in the problem size information */
Vscanf("%ld%ld%ld%ld%ld%*[\n] ", &n,
        &ncol, &nfv, &nrv, &nvpr);
nv = nfv + nrv;

/* Check problem size */
if (n < 0 || ncol < 0 || nfv < 0 || nrv < 0 || nvpr < 0)
{
Vprintf("Invalid problem size, at least one of n, ncol, nfv, nrv or nvpr"
        " is < 0\n");
exit_status = 1;
goto END;
}

/* Allocate memory first lot of memory */
if ( !(levels = NAG_ALLOC(ncol,Integer)) ||
    !(fvid = NAG_ALLOC(nfv,Integer)) ||
    !(rvid = NAG_ALLOC(nrv,Integer)) ||
    !(vpr = NAG_ALLOC(nrv, Integer)) )
{
Vprintf("Allocation failure\n");
exit_status = -1;
goto END;
}

/* Read in number of levels for each variable */
for (i = 1; i <= ncol; ++i)
{
Vscanf("%ld", &levels[i - 1]);
}
Vscanf("%*[\n] ");

/* Read in model information */
Vscanf("%ld", &yvid);
for (i = 1; i <= nfv; ++i)
{
Vscanf("%ld", &fvid[i - 1]);
}
for (i = 1; i <= nrv; i++)
{
Vscanf("%ld", &rvid[i - 1]);
}
Vscanf("%ld%ld%ld%ld%*[\n] ", &svid, &cwid,
        &fint, &rint);

/* Read in the variance component flag */
for (i = 1; i <= nrv; ++i)
{

```

```

        Vscanf("%ld", &vpr[i - 1]);
    }
    Vscanf("%*[^\\n] ");

/* If no subject specified, then ignore rint */
if (svid == 0)
{
    rint = 0;
}

/* Count the number of levels in the fixed parameters */
for (i = 1, fnlevel = 0; i <= nfv; ++i)
{
    fl = levels[fvid[i - 1] - 1] - 1;
    fnlevel += (fl < 1) ? 1 : fl;
}
if (fint == 1)
{
    fnlevel++;
}

/* Count the number of levels in the random parameters */
for (i = 1, rnlevel = 0; i <= nrv; ++i)
{
    rnlevel += levels[rvid[i - 1] - 1];
}
if (rint)
{
    rnlevel++;
}

/* Calculate the sizes of the output arrays */
if (rint == 1)
{
    lgamma = nvpr + 2;
}
else
{
    lgamma = nvpr + 1;
}
if (svid)
{
    lb = fnlevel + levels[svid-1] * rnlevel;
}
else
{
    lb = fnlevel + rnlevel;
}

tddat = ncol;

/* Allocate remaining memory */
if ( !(dat = NAG_ALLOC(n*ncol, double)) ||
      !(gamma = NAG_ALLOC(lgamma, double)) ||
      !(b = NAG_ALLOC(lb, double)) ||
      !(se = NAG_ALLOC(lb, double)))
{
    Vprintf("Allocation failure\\n");
    exit_status = -1;
    goto END;
}

/* Read in the Data matrix */
for (i = 1; i <= n; ++i)
{
    for (j = 1; j <= ncol; ++j)
    {
        Vscanf("%lf", &DAT(i,j));
    }
}

```

```

/* Read in the initial values for GAMMA */
for (i = 1; i < lgamma; ++i)
{
    Vscanf("%lf", &gamma[i - 1]);
}

/* Read in the maximum number of iterations */
Vscanf("%ld%*[\n] ", &maxit);

/* Run the analysis */
tol = 0.;
warnp = 0;
/* nag_ml_mixed_regsn (g02jbc).
 * Linear mixed effects regression using Maximum Likelihood
 * (ML)
 */
nag_ml_mixed_regsn(n, ncol, dat, tddat, levels, yvid, cwid, nfv, fvid, fint,
    nrv, rvid, nvpr, vpr, rint, svid, gamma, &nff, &nrf, &df,
    &like, lb, b, se, maxit, tol, &warnp, &fail);

/* Report the results */
if (fail.code == NE_NOERROR)
{
    /* Output results */
    if (warnp != 0)
    {
        Vprintf("%s", "Warning: At least one variance component was ");
        Vprintf("%s", "estimated to be negative and then reset to zero");
        Vprintf("\n");
    }
    Vprintf("%s\n\n", "Fixed effects (Estimate and Standard Deviation)");
    k = 1;
    if (fint == 1)
    {
        Vprintf("%s%10.4f%10.4f\n", "Intercept", b[k - 1],
            se[k - 1]);
        ++k;
    }
    for (i = 1; i <= nfv; ++i)
    {
        for (j = 1; j <= levels[fvid[i - 1] - 1]; ++j)
        {
            if (levels[fvid[i - 1] - 1] != 1 && j == 1) continue;
            Vprintf("%s%4ld%s%4ld%10.4f%10.4f\n", "Variable",
                i, " Level", j, b[k - 1], se[k - 1]);
            ++k;
        }
    }
    Vprintf("\n");
    Vprintf("%s\n", "Random Effects (Estimate and Standard", " Deviation)");
    if (svid == 0)
    {
        for (i = 1; i <= nrv; ++i)
        {
            for (j = 1; j <= levels[rvid[i - 1] - 1]; ++j)
            {
                Vprintf("%s%4ld%s%4ld%10.4f%10.4f\n",
                    "Variable", i, " Level", j, b[k - 1], se[k - 1]);
                ++k;
            }
        }
    }
    else
    {
        for (l = 1; l <= levels[svid - 1]; ++l)
        {
            if (rint == 1)
            {
                Vprintf("%s%4ld%s%10.4f%10.4f\n",

```

```

        "Intercept for Subject Level", l, " ",
        b[k - 1], se[k - 1]);
    ++k;
}
for (i = 1; i <= nrvc; ++i)
{
    for (j = 1; j <= levels[rvid[i - 1] - 1]; ++j)
    {
        Vprintf("%s%4ld%s%4ld%s%4ld"
                "%10.4f%10.4f\n", "Subject Level", l, " Variable",
                i, " Level", j, b[k - 1], se[k - 1]);
        ++k;
    }
}
}

Vprintf("\n");
Vprintf("%s\n", " Variance Components");
for (i = 1; i <= nvpr + rint; ++i)
{
    Vprintf("%4ld%10.4f\n", i, gamma[i - 1]);
}
Vprintf("%s%10.4f\n\n", "SIGMA^2", gamma[nvpr + rint]);

Vprintf("%s%10.4f\n\n", "-2LOG LIKE", like);
Vprintf("%s%ld\n", "DF", df);
}
else
{
    Vprintf("Routine nag_ml_mixed_regsn (g02jbc) failed, with error message:"
           "\n%s\n", fail.message);
}
}

END:
if (b) NAG_FREE(b);
if (dat) NAG_FREE(dat);
if (gamma) NAG_FREE(gamma);
if (se) NAG_FREE(se);
if (fvid) NAG_FREE(fvid);
if (levels) NAG_FREE(levels);
if (rvid) NAG_FREE(rvid);
if (vpr) NAG_FREE(vpr);
return exit_status;
}

```

## 9.2 Program Data

nag\_ml\_mixed\_regsn (g02jbc) Example Program Data

```

24 5 3 1 1
1 4 3 2 3
1 3 4 5 3 2 0 1 1
1
56 1 1 1 1
50 1 2 1 1
39 1 3 1 1
30 2 1 1 1
36 2 2 1 1
33 2 3 1 1
32 3 1 1 1
31 3 2 1 1
15 3 3 1 1
30 4 1 1 1
35 4 2 1 1
17 4 3 1 1
41 1 1 2 1
36 1 2 2 2
35 1 3 2 3
25 2 1 2 1
28 2 2 2 2

```

```

30 2 3 2 3
24 3 1 2 1
27 3 2 2 2
19 3 3 2 3
25 4 1 2 1
30 4 2 2 2
18 4 3 2 3
1.0 1.0
-1

```

### 9.3 Program Results

nag\_ml\_mixed\_regsn (g02jbc) Example Program Results

Fixed effects (Estimate and Standard Deviation)

Intercept			37.0000	4.0421
Variable	1 Level	2	1.0000	3.0461
Variable	1 Level	3	-11.0000	3.0461
Variable	2 Level	2	-8.2500	1.8736
Variable	3 Level	2	0.5000	2.6497
Variable	3 Level	3	7.7500	2.6497

Random Effects (Estimate and Standard Deviation)

Intercept for Subject Level	1		10.7631	3.8855	
Subject Level	1 Variable	1 Level	1	3.7276	2.6268
Subject Level	1 Variable	1 Level	2	-1.4476	2.6268
Subject Level	1 Variable	1 Level	3	0.3733	2.6268
Intercept for Subject Level	2		-0.5269	3.8855	
Subject Level	2 Variable	1 Level	1	-3.7171	2.6268
Subject Level	2 Variable	1 Level	2	-1.2253	2.6268
Subject Level	2 Variable	1 Level	3	4.8125	2.6268
Intercept for Subject Level	3		-5.6450	3.8855	
Subject Level	3 Variable	1 Level	1	0.5903	2.6268
Subject Level	3 Variable	1 Level	2	0.3987	2.6268
Subject Level	3 Variable	1 Level	3	-2.3806	2.6268
Intercept for Subject Level	4		-4.5912	3.8855	
Subject Level	4 Variable	1 Level	1	-0.6009	2.6268
Subject Level	4 Variable	1 Level	2	2.2742	2.6268
Subject Level	4 Variable	1 Level	3	-2.8052	2.6268

Variance Components

1	46.7969
2	11.5365
SIGMA <sup>2</sup>	= 7.0208
-2LOG LIKE	= 141.6877
DF	= 16

---