# THE INSTITUTE OF STATISTICS

**UNIVERSITY OF NORTH CAROLINA SYSTEM**

NLINVC USER'S GUIDE

Version 1b

by

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## ABSTRACT

The NLINVC macro procedure estimates parameters for nonlinear models with variance components by the method of estimated generalized least squares.

## INTRODUCTION

The NLINVC procedure estimates parameters for models of the form:

$$\mathbf{y} = \mathbf{f}(\mathbf{X},\boldsymbol{\beta}) + \sum_{i=1}^{k} \mathbf{U}_i \mathbf{e}_i$$

where $\mathbf{e}_1,\ldots,\mathbf{e}_k$ are independent random vectors with $E(\mathbf{e}_i)=0$ and $Var(\mathbf{e}_i)=\sigma_i^2\mathbf{I}$. The model for the mean, $\mathbf{f}(\mathbf{X},\boldsymbol{\beta})$ is nonlinear in the parameters and the parameters, $\boldsymbol{\beta}$, are all assumed to be fixed. The matrices, $\mathbf{U}_i$, correspond to random effects and are usually class variables such as replication or treatment x block. Each random effect, $\mathbf{U}_i$, is associated with a variance component, $\sigma_i^2$.

The parameters of the nonlinear mean model are estimated using the method of estimated generalized least squares (EGLS). The procedure follows a three part algorithm:

1) Obtain an initial estimate of $\boldsymbol{\beta}$ by the ordinary least squares (OLS) approach using a modified Gauss-Newton algorithm.
2) Fix $\boldsymbol{\beta}$ at the value obtained in step 1) and estimate the variance components using an approximate maximum likelihood method or an approximate restricted maximum likelihood method.
3) Using the estimated variance-covariance matrix from step 2), compute the estimated generalized least squares estimate of $\boldsymbol{\beta}$, again using a modified Gauss-Newton algorithm.

The user must specify the function for the mean model, initial values for the fixed parameters, partial derivatives of the mean function, a list of random factors, and the number of levels for each factor. Variance components can be estimated by approximate maximum likelihood or approximate restricted maximum likelihood. The user can also specify the number of iterations and adjust the convergence criterion for each step of the procedure. In addition to the printed output, NLINVC produces SAS data sets containing parameter estimates, variance components, predicted values and residuals.

NLINVC is written in the SAS macro facility. The syntax is similar, but not identical, to that of a regular SAS procedure. This program uses the SAS procedures NLIN, MIXMOD and IML; consequently the user has all the flexibility of NLIN for defining the mean function and doing auxiliary data manipulations. The required input follows that of PROCs NLIN and MIXMOD closely but not all options of those two procedures have been implemented in NLINVC.

## PRELIMINARIES

In order to run the program NLINVC, you must have a copy of the procedure MIXMOD and the data library NGUMP.NLINVC.MACAUTOS. At North Carolina State University the JCL for use with the program NLINVC is as follows:

```
//jobcard
// EXEC SAST,REGION=2000K,OPTIONS='MAUTOSOURCE IMPLMAC NOMRECALL'
//STEPLIB DD DSN=NFGG.MIXMOD.SAS0,DISP=SHR
//SASAUTOS DD DISP=SHR,DSN=NGUMP.NLINVC.MACAUTOS
//          DD DISP=SHR,DSN=SYSSAS.MACAUTOS.VERCUR
//any additional ddcards for input or output data sets
//SYSIN DD *
```

Please note that the SAS autocall library is called SYSSAS.MACAUTOS.VERCUR on the system at NCSU but may be called something else on your system. Explanation of the JCL can be found in the SAS Guide to Macro Processing, Version 5 Edition, especially page 144 and Appendix 2.

Two other preliminary steps must be taken before running NLINVC:

1) If the input data set has any missing values, delete those observations from the data set because NLINVC uses PROC IML heavily.
2) Issue a RUN command before issuing any NLINVC statements.

# SPECIFICATIONS

The following statements are part of the NLINVC macro procedure.

NLINVC options;

PARMINIT parameter=value parameter=value ...;

AUXIL programming statement, programming statement,...;

FUNCTION dependent=expression;

DERIV DERparameter=expression, DERparameter=expression, ...;

VOPTIONS options;

RANDOM random effects;

LVLS values;

PRIORVC values;

DATAOUT options;

RNLINVC;

**NLINVC statement**

NLINVC options;

The NLINVC statement is required. The options below can appear in the NLINVC statement:

DATA=SASdataset

names the SAS data set containing the data to be analyzed by macro procedure NLINVC. If DATA= is omitted, the most recently created SAS data set is used.

OUTEST=SASdataset

names the SAS data set to contain the parameter estimates produced by NLINVC. If OUTEST is omitted, the data set _BETA is used.

OUTVC=SASdataset

names the SAS data set to contain the variance component estimates produced by NLINVC. If OUTVC is omitted, the data set _VC is used.

MAXITER=i

places a limit on the number of iterations NLINVC performs in estimation of the fixed parameters. The i value must be a positive integer. The default is 30.

CONVERGE=c

specifies the relative convergence criterion. The iterations are said to have converged if (LASTSSE-SSE)/(SSE+10E-6) < c. The default is c=10E-8. The constant c should be a small positive number.

VBOLS=yes or no

specifies whether you want $\widehat{V}(\widehat{\beta}_{OLS})$ to be printed. The default is yes. Use the NO option if you have a large number of levels of the random effects or if you use the GROUPVAR option in the VOPTIONS statement.

**PARMINIT statement**

PARMINIT parameter=value ...;

A PARMINIT statement must follow the NLINVC statement. A parameter name and value must appear for every fixed parameter to be estimated. Specify only one value for each parameter. The parameter names must all be valid SAS names no longer than 5 characters and must not duplicate the names of any variables in the input data set. The values specify the starting values of the parameters.

**AUXIL statement**

AUXIL programming statement, programming statement, ...;

Any number of programming statements can be included in the AUXIL statement. Note that the programming statements are separated by commas, not semicolons. Use a semicolon to mark the end of the last programming statement. NLINVC can execute any statement that is acceptable to PROC NLIN, including assignment statements, IF statements and program control statements. For further details see the PROC NLIN description in the *SAS User's Guide: Statistics* (SAS Institute Inc. 1985).

**FUNCTION statement**

FUNCTION dependent=expression;

The FUNCTION statement declares the dependent variable and defines the function for the mean model. The expression can be any valid SAS expression and can include parameter names, variables in the input data set and variables created in the AUXIL statement. A FUNCTION statement must appear.

**DERIV statement**

DERIV DERparameter=expression, ...;

The DERIV statement must come after the PARMINIT statement. A derivative definition, DERparameter=expression, for each fixed parameter must appear in the DERIV statement. In each derivative definition the expression must be the algebraic representation of the partial derivative of the mean model given in the FUNCTION statement with respect to the parameter named in DERparameter. Separate the different derivative definitions with commas, and note that DERparameter has no period between DER and the parameter name, unlike PROC NLIN syntax.

**VOPTIONS statement**

VOPTIONS options;

The options below can appear in the VOPTIONS statement:

NORMALEQ=SASdataset

names the SAS data set which will contain the matrices involved in the normal equations for estimating $\boldsymbol{\beta}$. If NORMALEQ= is omitted, the normal equations are stored in the data set _NEQ.

VARIT=i

puts a limit on the number of iterations NLINVC performs to estimate the variance components. The i value must be a positive integer or zero. The default is 3. If VARIT=0, then variance component values must be specified using the PRIORVC statement.

GROUPVAR=grouping variable

estimates a separate residual variance for each group in the grouping variable. The data set must be previously sorted by the grouping variable. The option NUMGROUP must also be specified when GROUPVAR is used. If GROUPVAR is used, specify VBOLS=NO on the NLINVC statement.

NUMGROUP=g

gives the number of groups in the grouping variable. The GROUPVAR option must also be specified when NUMGROUP is used.

The following two options specify which method of estimation for variance components is desired. Only **one** of these options should be specified. If neither is specified, approximate maximum likelihood will be used for estimating the variance components.

VAREQMML=SASdataset

specifies that the method of estimating the variance components is approximate modified maximum likelihood and names the SAS dataset to contain the matrices used in the variance estimating equations, $\left(\left(\mathrm{tr}(\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{V}_j)\right)\right)$ and $\left(\left(\mathbf{y}'\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{y}\right)\right)$. If VAREQMML= is not specified, the matrices will be stored in the SAS data set _VEQMML.

VAREQML=SASdataset

specifies that the method of estimating the variance components is approximate maximum likelihood and names the SAS dataset to contain the matrices used in the variance estimating equations, $\left(\left(\mathrm{tr}(\hat{\mathbf{V}}^{-1}\mathbf{V}_i\hat{\mathbf{V}}^{-1}\mathbf{V}_j)\right)\right)$ and $\left(\left(\mathbf{y}'\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{y}\right)\right)$. If VAREQML= is not specified, the matrices will be stored in the SAS data set _VEQML.

**RANDOM statement**

RANDOM random effects;

The RANDOM statement lists the random effects in the model. The random effects are constructed from numeric variables in the input data set (note that variables must be numeric). Crossed and nested effects are both indicated by sets of variables joined by asterisks. Effects may be either discrete or continuous, but it is not possible to mix discrete and continuous variables in one effect, as in discrete*continuous. The rules for specifying effects follow the syntax for the MIXMOD MODEL statement. The RANDOM statement is required.

**LVLS statement**

LVLS values;

The LVLS statement specifies whether effects are continuous or discrete and specifies the maximum number of levels for each discrete effect. The model is stored with the fixed parameters of the nonlinear mean model first and the random effects following. The value list should include, in the order used in the PARMINIT and RANDOM statements, the number of levels for each effect in the model. Each fixed parameter in the nonlinear mean function is considered to be a continuous effect. Continuous effects are indicated by a 1 in the value list. For discrete effects the value should be the number of levels of the effect. See the MIXMOD LEVELS statement description for more details. If you use the GROUPVAR and NUMGROUP options then the levels should include the levels in the PARMINIT and RANDOM statements followed by the number of observations in each group. See the PRIORVC statement for an example.

**PRIORVC statement**

PRIORVC values;

The PRIORVC statement allows the user to give initial values for the variance components. This statement is optional. The default value is 1 for every variance component. The value list should include a value for every random effect in the model including the residual error. If the GROUPVAR option is used then there should be a value for the residual error for each group. Example:

3 parameters (A, B, and C) in the nonlinear model for the mean

2 random effects

location: 5 levels

block (location): 4 blocks for location 1; 3 blocks for other locations

10 observations per block except location 3, with 5 observations per block

prior values for variance components are $\sigma^2_{\text{loc}}=2$, $\sigma^2_{\text{block (loc)}}=3$, $\sigma^2_{\text{resid}}=1$

Case 1. Common residual variance for all observations

```
PARMINIT A=10 B=20 C=50;
:
VOPTIONS VAREQMML=VMML;
RANDOM LOC BLOCK*LOC;
LVLS 1 1 1 5 16;
PRIORVC 2 3 1;
```

Case 2. Separate residual variance for each location. Prior values are the same as above except residual variance for locations 4 and 5 is 1.5.

```
PARMINIT A=10 B=20 C=50;
:
VOPTIONS VAREQMML=VMML GROUPVAR=LOC NUMGROUP=5;
RANDOM LOC BLOCK*LOC;
LVLS 1 1 1 5 16 40 30 15 30 30;
PRIORVC 2 3 1 1 1 1.5 1.5;
```

**DATAOUT statement**

DATAOUT options;

The DATAOUT statement allows the user to specify a SAS data set name for the output data and variable names for the residuals and predicted values. The available options are:

OUT=SASdataset

names the SAS data set to be created by NLINVC. If OUT= is not specified, the output is stored in data set _OUT1. The new data set includes all variables in the input data set plus residuals, predicted values, auxiliary variables created with the AUXIL statement and derivatives.

R=variable name

names a variable in the output data set to contain the residuals. The variable name must be a valid SAS name and must not match any variable name in the input data set. If R= is not specified, the residuals are stored under the name _RESID.

P=variable name

names a variable in the output data set to contain the predicted values. The variable name must be a valid SAS name and must not match any variable name in the input data set. If P= is not specified, the predicted values are stored under the name _YHAT.

**RNLINVC statement**

RNLINVC;

The RNLINVC statement runs the macros that estimate the variance components and the fixed parameters. This statement is required and must come after all other NLINVC statements.

# STATISTICAL METHOD

In the nonlinear model with random components, $\mathbf{y} = \mathbf{f}(\mathbf{X},\boldsymbol{\beta}) + \sum_{i=1}^{k} \mathbf{U}_i\mathbf{e}_i$, where $\mathbf{e}_1,\ldots,\mathbf{e}_k$ are independent random vectors with $E(\mathbf{e}_i)=\mathbf{0}$ and Var $(\mathbf{e}_i)=\sigma_i^2\mathbf{I}$, $\mathbf{y}$ has the special covariance structure, $\mathbf{V}=\mathrm{Var}(\mathbf{y})=\sum_{i=1}^{k}\mathbf{V}_i\sigma_i^2$, where $\mathbf{V}_i = \mathbf{U}_i\mathbf{U}_i'$. An estimated generalized least squares estimator, $\hat{\boldsymbol{\beta}}_{\mathrm{GLS}}$, is defined as any vector that minimizes the sum of squares, $(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))$ with respect to $\boldsymbol{\beta}$, where $\hat{\mathbf{V}}$ is some previously computed estimate of $\mathbf{V}$. If $\hat{\mathbf{V}}$ is a strongly consistent estimator for $\mathbf{V}$, then this estimator is strongly consistent for $\boldsymbol{\beta}$ and asymptotically normal and efficient under certain regularity conditions. It has the same asymptotic distribution as the generalized least squares estimator, which minimizes $(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))$ if $\mathbf{V}$ is known.

There are many possible methods for obtaining an EGLS estimator, each differing in the way the covariance matrix, $\mathbf{V}$, is estimated. However all follow a three part algorithm.

1) Obtain an initial estimate, $\hat{\boldsymbol{\beta}}_0$, of the fixed parameters.

2) Estimate the variance-covariance matrix, $\mathbf{V}$.

3) Minimize $\mathrm{SSE}=(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))$ to obtain a final estimate, $\hat{\boldsymbol{\beta}}_{\mathrm{EGLS}}$.

In the macro procedure NLINVC the initial estimate, $\hat{\boldsymbol{\beta}}_0$, of the fixed parameter vector, $\boldsymbol{\beta}$, is computed using ordinary nonlinear least squares. For this first step the error structure represented by the random effects is ignored and the unweighted residual sums of squares, $(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))$, is minimized. This initial fitting is carried out in PROC NLIN with the option METHOD=GAUSS.

The variance components, $\sigma_i^2$, are estimated based on the residuals, $\mathbf{r}_0 = \mathbf{y} - \mathbf{f}(\mathbf{X},\hat{\boldsymbol{\beta}}_0)$, from the initial estimate of $\boldsymbol{\beta}$. Under the assumption of normally distributed random effects, the log of the likelihood function is

$$L = \text{constant} - \tfrac{1}{2}\ln|\mathbf{V}| - \tfrac{1}{2}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta})).$$

Consider the linear approximation of the mean function obtained by Taylor series expansion,

$$\mathbf{f}(\mathbf{X},\boldsymbol{\beta}) \doteq \mathbf{f}(\mathbf{X},\hat{\boldsymbol{\beta}}_0) + \frac{\partial\mathbf{f}(\mathbf{X},\hat{\boldsymbol{\beta}}_0)}{\partial\boldsymbol{\beta}'}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}_0).$$

Define $\mathbf{D_0} = \dfrac{\partial \mathbf{f}(\mathbf{X},\hat{\boldsymbol\beta}_0)}{\partial \boldsymbol\beta'}$ and $\boldsymbol\delta_0 = \boldsymbol\beta - \hat{\boldsymbol\beta}_0$. Then an approximate log likelihood function which can be maximized with respect to $\boldsymbol\beta$ and $\sigma_i^2$, i=1,...,k is

$$L \doteq \text{constant} - \tfrac{1}{2}\ln|\mathbf{V}| - \tfrac{1}{2}(\mathbf{r_0} - \mathbf{D_0}\boldsymbol\delta)'\mathbf{V}^{-1}(\mathbf{r_0} - \mathbf{D_0}\boldsymbol\delta).$$

Using the special structure of the covariance matrix, $\mathbf{V}=\sum_{i=1}^{k}\mathbf{V}_i\sigma_i^2$, this equation can be maximized iteratively by a method adapted from Hemmerle and Hartley's (1973) method for linear variance components models, which yields the following estimating equations:

$$\left(\left(\text{trace}(\mathbf{V}_i\mathbf{V}_{(h)}^{-1}\mathbf{V}_j\mathbf{V}_{(h)}^{-1})\right)\right)\left(\left(\hat\sigma^2_{j(h+1)}\right)\right) = \left(\left(\mathbf{r_0}'\mathbf{Q}_{(h)}\mathbf{V}_i\mathbf{Q}_{(h)}\mathbf{r_0}\right)\right),$$

where h indicates the iteration number, oversize double parentheses indicate a matrix with elements of the enclosed form, and

$$\mathbf{Q}_{(h)} = \mathbf{V}_{(h)}^{-1}(\mathbf{I} - \mathbf{D_0}(\mathbf{D_0}'\mathbf{V}_{(h)}^{-1}\mathbf{D_0})^{+}\mathbf{D_0}'\mathbf{V}_{(h)}^{-1}),$$

where $(\ )^{+}$ indicates a generalized inverse. Solutions to these equations, achieved when further iteration does not increase the log likelihood, may not be positive, in which case they are reset to zero before the next iteration. These equations are iteratively produced by PROC MIXMOD and solved in PROC IML until either the convergence criterion is satisfied or the maximum number of iterations specified is reached. The approximate covariance matrix of the variance components, based on the variance of a quadratic form of a normally distributed random vector with mean zero, is computed as:

$$\hat{\mathbf{V}}\left(\left(\hat\sigma_i^2\right)\right) = 2\left(\left(\text{trace}(\hat{\mathbf{V}}^{-1}\mathbf{V}_i\hat{\mathbf{V}}^{-1}\mathbf{V}_j)\right)\right)\left(\left(\text{trace}(\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{V}_j)\right)\right)\left(\left(\text{trace}(\hat{\mathbf{V}}^{-1}\mathbf{V}_i\hat{\mathbf{V}}^{-1}\mathbf{V}_j)\right)\right),$$

where $\hat{\mathbf{V}}$ is the final estimate of $\mathbf{V}$.

Variance components can also be estimated by approximate modified maximum likelihood, in which the likelihood function is based on vectors in the error space, that is, on linear combinations of $\mathbf{y}$ which have expectation zero, rather than on $\mathbf{y}$ itself. The macro procedure NLINVC uses the linear approximation $\mathbf{r_0} \doteq \mathbf{D_0}\boldsymbol\delta + \mathbf{e}$ to obtain vectors in the error space. Vectors of the form $\mathbf{k}'\mathbf{y}$, where $\mathbf{k}$ is chosen so that $\mathbf{k}'\mathbf{D_0} = \mathbf{0}$, then fall in this linear approximation to the error space. The log likelihood function of $\mathbf{K}'\mathbf{y}$, where $\mathbf{K}$ is a full rank matrix of vectors $\mathbf{k}$, is:

$$L = \text{constant} - \tfrac{1}{2}\ln|\mathbf{K}'\mathbf{V}\mathbf{K}| - \tfrac{1}{2}(\mathbf{K}'\mathbf{y} - \mathbf{K}'\mathbf{f}(\mathbf{X},\boldsymbol\beta))'(\mathbf{K}'\mathbf{V}\mathbf{K})^{-1}(\mathbf{K}'\mathbf{y} - \mathbf{K}'\mathbf{f}(\mathbf{X},\boldsymbol\beta)),$$

which is approximated by:

$$L \doteq \text{constant} - \tfrac{1}{2}\ln|\mathbf{K}'\mathbf{V}\mathbf{K}| - \tfrac{1}{2}\mathbf{r_0}'\mathbf{K}(\mathbf{K}'\mathbf{V}\mathbf{K})^{-1}\mathbf{K}'\mathbf{r_0}.$$

This restricted likelihood function can be maximized by iteratively solving the system of equations:

$$\left(\left(\text{trace}(\mathbf{Q}_{(h)}\mathbf{V}_i\mathbf{Q}_{(h)}\mathbf{V}_j)\right)\right)\left(\left(\hat{\sigma}^2_{j(h+1)}\right)\right) = \left(\left(\mathbf{y}'\mathbf{Q}_{(h)}\mathbf{V}_i\mathbf{Q}_{(h)}\mathbf{y}\right)\right).$$

As in the approximate maximum likelihood algorithm, if this procedure results in any negative variance estimate, that variance component is set to zero and then iterations are resumed. For modified maximum likelihood the covariance matrix of the variance components is approximately

$$\hat{\mathbf{V}}\left(\left(\hat{\sigma}^2_i\right)\right) = 2\left(\left(\text{trace}(\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{V}_j)\right)\right).$$

Finally, $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$ is computed using a modified Gauss-Newton algorithm to minimize SSE=$(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\boldsymbol{\beta}))$ with respect to $\boldsymbol{\beta}$. The variance components, $\hat{\sigma}^2_i$, obtained in the previous step are used to form $\hat{\mathbf{V}}=\sum_{i=1}^{k}\mathbf{V}_i\hat{\sigma}^2_i$. The Gauss-Newton algorithm for generalized least squares is similar to that for ordinary least squares, essentially approximating the sum of squares surface with the ellipsoid $(\mathbf{r_0} - \mathbf{D_0}\hat{\boldsymbol{\delta}})'\hat{\mathbf{V}}^{-1}(\mathbf{r_0} - \mathbf{D_0}\hat{\boldsymbol{\delta}})$. The approximate normal equations, $\mathbf{D_0}'\hat{\mathbf{V}}^{-1}\mathbf{D_0}\hat{\boldsymbol{\delta}} = \mathbf{D_0}'\hat{\mathbf{V}}^{-1}\mathbf{r_0}$, are solved, then the program checks to ensure that the new sum of squares, $\text{SSE}_{(1)} = (\mathbf{y} - \mathbf{f}(\mathbf{X},\hat{\boldsymbol{\beta}}_{(1)}))'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{X},\hat{\boldsymbol{\beta}}_{(1)}))$ is less than $\text{SSE}_{(0)}$. If it is not, the update vector $\hat{\boldsymbol{\delta}}$ is halved (up to ten times) until SSE is smaller than $\text{SSE}_{(0)}$. These approximate normal equations are produced by PROC MIXMOD, solved in PROC IML and the process is iterated until convergence. If the convergence criterion is satisfied or if halving $\boldsymbol{\delta}$ does not provide any improvement, so that SSE is assumed to be at a minimum, the standard errors and Wald-type confidence intervals, $\hat{\boldsymbol{\beta}} \pm \text{t}(.975,\text{df})\text{se}(\hat{\boldsymbol{\beta}})$, of the fixed parameter estimates are printed out. The variance-covariance matrix of $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$ is estimated as

$$\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}_{\text{EGLS}}) = (\hat{\mathbf{D}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{D}})^{-1},$$

where $\hat{\mathbf{D}}$ indicates the matrix of partial derivatives evaluated at $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$.

The estimated standard errors for the ordinary least squares estimates are also printed. If the estimates of the variance components have high variance, for instance if they are computed based on a small number of replicates, then $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ may be preferred over $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$. In this case the variance-covariance matrix of $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ is estimated as

$$\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}_{\text{OLS}}) = (\mathbf{D_0}'\mathbf{D_0})^{-1}\mathbf{D_0}'\hat{\mathbf{V}}\mathbf{D_0}(\mathbf{D_0}'\mathbf{D_0})^{-1},$$

where the partial derivatives are computed using $\hat{\boldsymbol{\beta}}_{\text{OLS}}$. If, on the other hand, the variance components are estimated well, then $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$ has smaller variance than the ordinary least squares estimator. In this case the variance-covariance matrix of $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ can be estimated as

$$\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}_{\text{OLS}}) = (\hat{\mathbf{D}}'\hat{\mathbf{D}})^{-1}\hat{\mathbf{D}}'\hat{\mathbf{V}}\hat{\mathbf{D}}(\hat{\mathbf{D}}'\hat{\mathbf{D}})^{-1},$$

where the matrix of partial derivatives is evaluated at $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$. Then the estimated standard error of $\hat{\boldsymbol{\beta}}_{\text{OLS}}$ based on this covariance estimate can be compared to the estimated standard error of $\hat{\boldsymbol{\beta}}_{\text{EGLS}}$ to get an indication of how much precision is gained by using estimated generalized least squares over ordinary nonlinear least squares.

# DETAILS

**NLINVC Output**

The three steps of the EGLS algorithm each produce output. The first step prints the title 'INITIAL ESTIMATE OF FIXED PARAMETERS USING OLS' at the top of each page. The output from this step is produced by PROC NLIN and the user should be aware that the estimated standard errors and correlation matrix produced by PROC NLIN are not correct for the nonlinear model with variance components. The correct asymptotic standard errors for $\hat{\beta}_{OLS}$ appear in the output for step 3. The second step has pages entitled 'ESTIMATE VARIANCE COMPONENTS' and the third step of the procedure has pages entitled 'ESTIMATE FIXED PARAMETERS'.

**Troubleshooting**

NLINVC contains macro invocations, so in general it will be necessary to print the SAS statements generated by the macros in order to pinpoint where an error has occurred. This is accomplished by using the options MPRINT and SYMBOLGEN either in an OPTIONS statement or on the EXEC SAS card. Use of these options generates several pages of log output. Even without these options, the log produced by NLINVC may be longer than desired. It can be reduced somewhat by using the NONOTES option.

NLINVC may take more time than the default time limit. Experience indicates that TIME=1 will often be a good starting value.

**Global Macro Variables**

The following global macro variables are created by NLINVC commands. If any user-defined macro variables are given names from this list prior to running NLINVC unexpected results may occur. The contents of these macro variables are available to the user after running NLINVC.

| Variable Name | Contents | Default |
|---|---|---|
| INDATA | name of input data set | current |
| EST | name of data set to store $\hat{\beta}$ | _BETA |
| VC | name of data set to store $\hat{\sigma}_i^2$ | _VC |
| MAXIT | number of iterations for estimating $\beta$ | 30 |
| EPSBETA | convergence criterion for $\beta$ | 10E-8 |

| Variable Name | Contents | Default |
|---|---|---|
| PARMNAME | list of parameter names | |
| DERLIST | list of parameter names with prefix DER | |
| NF | number of fixed parameters | |
| PARMDEF | list of initial parameter definitions (parameter=value parameter=value ...) | |
| AUXILDEF | programming statements to perform auxiliary data manipulations (statement 1; statement 2; ...) | |
| FNDEF | mean function definition (dependent=expression) | |
| DERDEF | derivative definitions (DERparameter=expression; ...) | |
| OUTDATA | name of output data set for data, residuals and predicted values | _OUTDATA |
| RESID | name of variable to store residuals | _RESID |
| PRED | name of variable to store pred. values | _YHAT |
| NORMEQ | data set name to store normal equations | _NEQ |
| VAREQ | data set name for var. est. equations | _VEQML |
| VMETHOD | var. component est. method (ML or MML) | ML |
| VARITER | number of iterations for estimating $\hat{\sigma}_i^2$ | 3 |
| VEQMML | data set name for MML var. est. equations | _VEQMML |
| VEQML | data set name for ML var. est. equations | _VEQML |
| GROUPS | grouping variable | |
| NG | number of groups | |
| GRINFO | contains MIXMOD OPTIONS "GROUP=&GROUPS KE=&NG" | |
| ULIST | list of random effects | |
| NR | number of random effects (incl. residuals) | |
| ULISTQ | ULIST with each term enclosed in quotes | |
| UVARLIST | list of variables included in random effects | |
| ERROR | resid1 ... resid&NG | |

**Data Sets Created by NLINVC**

The NLINVC statement options create the following data sets. Examples of these data sets are provided in the next section. In all cases the data sets are created regardless of whether or not the user specifies names for them. The default data set names are given in parentheses. For more information about the NORMALEQ=, VAREQMML= and VAREQML= data sets see the MIXMOD user guide (Giesbrecht 1985).

| statement | option (default dsname) | contents |
|---|---|---|
| NLINVC | OUTEST=(_BETA) | parameter estimates, update vector, $\boldsymbol{\delta}$, and SSE from all iterations |
| NLINVC | OUTVC=(_VC) | variance component estimates from all iterations |
| DATAOUT | OUT=(_OUT1) | input variables, auxiliary variables, derivatives evaluated at $\hat{\beta}_{EGLS}$, predicted values and residuals |
| VOPTIONS | NORMALEQ=(_NEQ) | columns of $\hat{\mathbf{D}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{D}}$ (labeled XVIX) and $\hat{\mathbf{D}}'\hat{\mathbf{V}}\hat{\mathbf{r}}$ (labeled XVIY), n (last entry of XVIX_001) and $\hat{\mathbf{r}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{r}}$ (last entry in XVIY) |
| VOPTIONS | VAREQMML=(_VEQMML) | columns of $\left(\left(\mathrm{tr}\ \hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{V}_j\right)\right)$ (labeled QVQV) and $\left(\left(\mathbf{y}'\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{y}\right)\right)$ (labeled YQVQY); values of the variance components and the ln(likelihood) are stored in that order in the row labeled PRIORS |

| statement | option (default dsname) | contents |
|---|---|---|
| VOPTIONS | VAREQML=(_VEQML) | columns of $\left(\left(\text{tr } \hat{\mathbf{V}}^{-1}\mathbf{V}_i\hat{\mathbf{V}}^{-1}\mathbf{V}_j\right)\right)$ (labeled MLEQ) and $\left(\left(\mathbf{y}'\hat{\mathbf{Q}}\mathbf{V}_i\hat{\mathbf{Q}}\mathbf{y}\right)\right)$ (labeled YQVQY); values of variance components and the ln(likelihood) are stored in that order in the row labeled PRIORS |

The following data sets are created by the RNLINVC statement and the user does not have the option of naming them. Except for the data set _OUT0, they store results of the last iteration only.

| data set | contents |
|---|---|
| _OUT0 | input variables, auxiliary variables, derivatives, predicted values, and residuals evaluated at $\hat{\beta}_{\text{OLS}}$ |
| _SIG2 | variance component estimates |
| _VCI | variance components and ln(likelihood) |
| _SSEI | SSE |
| _BETAI | parameter estimates and update values, $\boldsymbol{\delta}$ |

# CHANGES FROM VERSION 1A

1. Add option for suppressing printout of $V(\widehat{\beta}_{\text{OLS}})$. If the number of levels of random effects is very large IML runs out of space.

   Old: $V(\widehat{\beta}_{\text{OLS}})$ computed automatically.

   New: VBOLS=(yes or no) option added to the NLINVC statement. Default is VBOLS=YES.

2. Make AUXIL, PRIORVC, and DATAOUT statements optional.

Old: AUXIL, PRIORVC, and DATAOUT statments were required.

New: These three statements can be omitted.

Default for PRIORVC is 1 for every variance component.

Default for DATAOUT is OUTDATA=_OUT1 R=_RESID P=_YHAT.

3. Add option for different within-group variances for different groups.

Old: All groups were assumed to have common within-group variance.

New: Options GROUPVAR=(name of grouping variable) and NUMGROUP=(number of groups) have been added to the VOPTIONS statement.

Default is NUMGROUP=1.

When you use these options the data must be sorted by groups and both options must be used together. Furthermore, you must declare the number of levels in each group on the LVLS statement. Example: 2 parameters in the model for the mean, 5 sites (random), 3 blocks per site, different within-block variance for each site. Sort data by site then use

```
VOPTIONS GROUPVAR=SITE NUMBGROUP=5;
RANDOM SITE BLOCK*SITE;
LVLS 1 1 5 15 n1 n2 n3 n4 n5;
```

where ni is the number of observations at the ith site.

If you are using the PRIORVC statement, then the list of prior variance components must include a value for the residual variance for each group.

```
PRIORVC vc(site)  vc(block*site) vc(error, site1) ... vc(error, site5);
```

4. Allow user to specify variance components to be used in EGLS.

Old: NLINVC automatically estimates the variance components iteratively.

New: Can specify VARIT=0 on the VOPTIONS statement. If this option is used, the variance components specified with the PRIORVC statement are used as is for estimating the fixed parameters. The PRIORVC statement must be used when VARIT=0.

# EXAMPLE

**Weibull Curve with Random Year and Block Effects**

This example demonstrates use of NLINVC for combining data from different experiments. Studies of the effect of ozone exposure on soybean yield were conducted in 1982, 1984 and 1986. In two of the years randomized block designs were used, but in the third year the experiment was completely randomized. The experiments differed further in that only one moisture treatment was used in 1982 (well watered); in 1984 a second moisture treatment was added (water stressed); and in 1986 a third moisture treatment involving rain exclusion caps was added. In this example the effect of ozone exposure (x) on soybean yield (y) is modelled with a Weibull curve with separate intercept parameters ($\alpha$) for different watering regimes. Year and block(year) are included as random effects. The model for the $i^{th}$ year, the $j^{th}$ block within year and the $k^{th}$ plot within a block is:

$$y_{ijk}=(\alpha+ \alpha_2 mdum_{2ijk}+\alpha_3 mdum_{3ijk})\exp\{-(x_{ijk}/w)^{\lambda}\}+e_{1i}+e_{2ij}+e_{3ijk}$$

where $mdum_2$ and $mdum_3$ are dummy variables for the second and third moisture treatments, $e_{1i}$ is the year effect, $e_{2ij}$ is the block(year) effect and $e_{3ijk}$ is the within-block error.

```
OPTIONS NONOTES;
DATA SOYBEAN;
  INFILE DATA;
  INPUT ID $ CULTIVAR $ BLOCK OZONE $ SULFUR $ MOISTURE $ O7HR O12HR SO2 KG_HA SEEDWT COV;
  Y=SQRT(KG_HA);
  IF ID='R82SO' THEN DO;
    YEAR=2; BLK=BLOCK; END;
  IF ID='R84SO' THEN DO;
    YEAR=4; BLK=BLOCK; END;
  IF ID='R86SO' THEN DO;
    YEAR=6; BLK=1;  END;
  MDUM1=(MOISTURE='-');
  MDUM2=(MOISTURE='+');
  MDUM3=(MOISTURE='T');
  RENAME O12HR=X;
  DROP ID CULTIVAR BLOCK OZONE SULFUR O7HR SO2 KG_HA SEEDWT COV;

PROC PRINT DATA=SOYBEAN;
```

| OBS | MOISTURE | X | Y | YEAR | BLK | MDUM1 | MDUM2 | MDUM3 |
|---|---|---|---|---|---|---|---|---|
| 1 | + | 0.054 | 60.0833 | 2 | 1 | 0 | 1 | 0 |
| 2 | + | 0.065 | 56.6701 | 2 | 1 | 0 | 1 | 0 |
| 3 | + | 0.081 | 50.5791 | 2 | 1 | 0 | 1 | 0 |
| ⋮ | | | | | | | | |
| 69 | T | 0.088 | 67.3976 | 6 | 1 | 0 | 0 | 1 |

```
RUN;
NLINVC MAXITER=10;
  PARMINIT ALPHA=75 AM2=50 AM3=50 OMEGA=0.10 LAMBD=2;
  AUXIL
    E=EXP(-(X/OMEGA)**LAMBD),
    F=(ALPHA+AM2*MDUM2+AM3*MDUM3)*E;
  DERIV
    DERALPHA=E, DERAM2=MDUM2*E, DERAM3=MDUM3*E,
    DEROMEGA=F*(LAMBD/OMEGA)*((X/OMEGA)**LAMBD),
    DERLAMBD= −F*((X/OMEGA)**LAMBD)*LOG(X/OMEGA);
  FUNCTION Y=F;
  DATAOUT OUT=OUTDATA R=RESID P=YHAT;
  VOPTIONS NORMALEQ=NEQ VAREQML=VEQ VARIT=5;
  RANDOM YEAR YEAR*BLK;
  LVLS 1 1 1 1 1 3 5;
  PRIORVC 1 1 1;
  RNLINVC;
PROC PRINT DATA=_BETA; TITLE 'LIST DATA SET _BETA';
PROC PRINT DATA=_VC; TITLE 'LIST DATA SET _VC';
PROC PRINT DATA=OUTDATA; TITLE 'LIST DATA SET OUTDATA';
PROC PRINT DATA=NEQ; TITLE 'LIST DATA SET NEQ';
PROC PRINT DATA=VEQ; TITLE 'LIST DATA SET VEQ';
PROC PRINT DATA=_VEQMML; TITLE 'LIST DATA SET _VEQMML';
```

INITIAL ESTIMATE OF FIXED PARAMETERS USING OLS

NON-LINEAR LEAST SQUARES ITERATIVE PHASE

DEPENDENT VARIABLE: Y METHOD: GAUSS-NEWTON

| ITERATION | ALPHA | AM2 | AM3 | OMEGA | LAMBD | RESIDUAL SS |
|---|---|---|---|---|---|---|
| 0 | 75.0000 | 50.0000 | 50.0000 | 0.1000 | 2.0000 | 49628.335919008 |
| 1 | 77.0177 | 1.3382 | 19.9920 | 0.1261 | 1.3341 | 8666.514323055 |
| 2 | 77.9718 | 3.2105 | 21.3487 | 0.1756 | 0.9175 | 7292.033800502 |
| 3 | 78.7180 | 3.0706 | 21.4851 | 0.2214 | 0.8762 | 6041.735933834 |
| 4 | 78.8261 | 3.0514 | 21.4986 | 0.2344 | 0.8694 | 5992.522121252 |
| 5 | 78.8841 | 3.0466 | 21.5098 | 0.2356 | 0.8663 | 5992.391782962 |
| 6 | 78.8750 | 3.0458 | 21.5076 | 0.2355 | 0.8668 | 5992.391738169 |

NOTE: CONVERGENCE CRITERION MET.

NON-LINEAR LEAST SQUARES SUMMARY STATISTICS DEP VARIABLE Y

| SOURCE | DF | SUM OF SQUARES | MEAN SQUARE |
|---|---|---|---|
| REGRESSION | 5 | 286259.49326 | 57251.89865 |
| RESIDUAL | 64 | 5992.39174 | 93.63112 |
| UNCORR TOTAL | 69 | 292251.88500 | |
| (CORR TOTAL) | 68 | 10802.76591 | |

| PARAMETER | ESTIMATE | ASYMPTOTIC STD. ERROR | ASYMPTOTIC 95 % CONFIDENCE INTERVAL LOWER | UPPER |
|---|---|---|---|---|
| ALPHA | 78.87495533 | 16.441819370 | 46.028610878 | 111.72129978 |
| AM2 | 3.04582683 | 3.467822112 | -3.881951484 | 9.97360513 |
| AM3 | 21.50755168 | 5.779685044 | 9.961291409 | 33.05381195 |
| OMEGA | 0.23549555 | 0.132140182 | -0.028485083 | 0.49947619 |
| LAMBD | 0.86677640 | 0.825411199 | -0.782173747 | 2.51572656 |

INITIAL ESTIMATE OF FIXED PARAMETERS USING OLS

ASYMPTOTIC CORRELATION MATRIX OF THE PARAMETERS

| CORR | ALPHA | AM2 | AM3 | OMEGA | LAMBD |
|---|---|---|---|---|---|
| ALPHA | 1.0000 | -.0092 | .4588 | .8052 | -.9591 |
| AM2 | -.0092 | 1.0000 | .4509 | .1110 | -.1263 |
| AM3 | .4588 | .4509 | 1.0000 | .4462 | -.5320 |
| OMEGA | .8052 | .1110 | .4462 | 1.0000 | -.9279 |
| LAMBD | -.9591 | -.1263 | -.5320 | -.9279 | 1.0000 |

## ESTIMATE VARIANCE COMPONENTS

| VCRECORD | ITERATION | YEAR | YEAR*BLK | ERROR | LNLR |
|---|---|---|---|---|---|
| | 0 | 1 | 1 | 1 | -522.775 |
| | 1 | 66.08578 | 9.849002 | 11.76968 | -192.098 |
| | 2 | 85.66606 | 0.8973977 | 11.79198 | -191.069 |
| | 3 | 89.84488 | 0.478754 | 11.77929 | -191.047 |
| | 4 | 89.98436 | 0.5181502 | 11.77074 | -191.046 |
| CONVERGENCE CRITERION MET | 5 | 89.98599 | 0.5133806 | 11.77174 | -191.046 |

## APPROXIMATE COVARIANCE MATRIX OF THE VARIANCE COMPONENTS

| VARVC | YEAR | YEAR*BLK | ERROR |
|---|---|---|---|
| YEAR | 3658.475 | -1.99244 | 0.2788725 |
| YEAR*BLK | -1.99244 | 2.98767 | -0.409736 |
| ERROR | 0.2788725 | -0.409736 | 4.056032 |

ESTIMATE FIXED PARAMETERS

| SUM-MARY | ITER | SUBIT | ALPHA | AM2 | AM3 | OMEGA | LAMBD | SSE |
|---|---|---|---|---|---|---|---|---|
| ROW1 | 0 | 0 | 78.8750 | 3.0458 | 21.5076 | 0.2355 | 0.8668 | 182.17503 |
| ROW2 | 1 | 0 | 46.6501 | 5.6031 | 1.0128 | 0.00206 | 2.4086 | 474.56634 |
| ROW3 | 1 | 1 | 62.7625 | 4.3244 | 11.2602 | 0.1188 | 1.6377 | 110.83753 |
| ROW4 | 2 | 0 | 63.6058 | 6.0229 | 6.7815 | 0.1362 | 2.2739 | 75.742882 |
| ROW5 | 3 | 0 | 66.8697 | 5.7957 | 7.3275 | 0.1300 | 2.3219 | 72.667594 |
| ROW6 | 4 | 0 | 66.7780 | 5.8108 | 7.3489 | 0.1306 | 2.3140 | 72.649527 |
| ROW7 | 5 | 0 | 66.7854 | 5.8088 | 7.3470 | 0.1306 | 2.3153 | 72.649506 |
| ROW8 | 6 | 0 | 66.7874 | 5.8088 | 7.3469 | 0.1306 | 2.3148 | 72.649504 |

CONVERGENCE CRITERION MET

| PARAM | ESTIMATE | STD ERROR | LCL95 | UCL95 |
|---|---|---|---|---|
| ALPHA | 66.78744680 | 5.77652861 | 55.24750365 | 78.32738994 |
| AM2 | 5.80878848 | 1.20617598 | 3.39917482 | 8.21840215 |
| AM3 | 7.34685956 | 1.66245165 | 4.02573041 | 10.66798872 |
| OMEGA | 0.13064281 | 0.01195526 | 0.10675943 | 0.15452618 |
| LAMBD | 2.31479635 | 0.39104709 | 1.53358994 | 3.09600276 |

ASYMPTOTIC CORRELATION MATRIX OF THE PARAMETERS

| CORRB | ALPHA | AM2 | AM3 | OMEGA | LAMBD |
|---|---|---|---|---|---|
| ALPHA | 1.0000 | -.1866 | -.1280 | .5892 | -.2562 |
| AM2 | -.1866 | 1.0000 | .3696 | -.02156 | -.01085 |
| AM3 | -.1280 | .3696 | 1.0000 | -.03725 | .01458 |
| OMEGA | .5892 | -.02156 | -.03725 | 1.0000 | -.8498 |
| LAMBD | -.2562 | -.01085 | .01458 | -.8498 | 1.0000 |

ESTIMATE FIXED PARAMETERS

ASYMPTOTIC STANDARD ERRORS AND CORRELATION MATRIX

OF ORDINARY LEAST SQUARES ESTIMATE, BOLS

1) COMPUTED USING DERIVATIVES EVALUATED AT BOLS

| PARAM | EST | STD ERROR | CORR | ALPHA | AM2 | AM3 | OMEGA | LAMBD |
|---|---|---|---|---|---|---|---|---|
| ALPHA | 78.8750 | 20.3897 | ALPHA | 1.000 | -.404 | .820 | .921 | .920 |
| AM2 | 3.0458 | 6.3358 | AM2 | -.404 | 1.000 | .016 | -.089 | .140 |
| AM3 | 21.5076 | 12.4844 | AM3 | .820 | .016 | 1.000 | .932 | -.952 |
| OMEGA | 0.2355 | 0.1450 | OMEGA | .921 | -.089 | .932 | 1.000 | -.980 |
| LAMBD | 0.8668 | 0.9448 | LAMBD | -0.920 | .140 | -.952 | -.980 | 1.000 |

2) COMPUTED USING DERIVATIVES EVALUATED AT BEGLS

| PARAM | EST | STD ERROR | CORR | ALPHA | AM2 | AM3 | OMEGA | LAMBD |
|---|---|---|---|---|---|---|---|---|
| ALPHA | 78.8750 | 8.5446 | ALPHA | 1.000 | -.683 | .227 | .572 | -.529 |
| AM2 | 3.0458 | 5.5764 | AM2 | -.683 | 1.000 | .087 | -.251 | .299 |
| AM3 | 21.5076 | 7.6719 | AM3 | .227 | .087 | 1.000 | .870 | -.862 |
| OMEGA | 0.2355 | 0.0384 | OMEGA | .572 | -.251 | .870 | 1.000 | -.985 |
| LAMBD | 0.8668 | 1.3880 | LAMBD | -.529 | .299 | -.862 | -.985 | 1.000 |

LIST DATA SET _BETA

| OBS | ALPHA | AM2 | AM3 | OMEGA | LAMBD | OLD1 | DELTA1 | OLD2 | DELTA2 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 78.875 | 3.0458 | 21.508 | 0.236 | 0.8668 | . | . | . | . |
| 2 | 46.650 | 5.6031 | 1.013 | 0.002 | 2.4086 | 78.8750 | -32.225 | 3.04583 | 2.5572 |
| 3 | 62.763 | 4.3244 | 11.260 | 0.119 | 1.6377 | 78.8750 | -16.112 | 3.04583 | 1.2786 |
| 4 | 63.606 | 6.0229 | 6.782 | 0.136 | 2.2740 | 62.7625 | 0.843 | 4.32444 | 1.6984 |
| 5 | 66.870 | 5.7957 | 7.328 | 0.130 | 2.3219 | 63.6058 | 3.264 | 6.02285 | -0.2272 |
| 6 | 66.778 | 5.8108 | 7.349 | 0.131 | 2.3140 | 66.8697 | -0.092 | 5.79569 | 0..0151 |
| 7 | 66.785 | 5.8088 | 7.347 | 0.131 | 2.3153 | 66.7780 | 0.007 | 5.81082 | -0.0020 |
| 8 | 66.787 | 5.8088 | 7.347 | 0.131 | 2.3148 | 66.7854 | 0.002 | 5.80883 | -0.0000 |

| OBS | OLD3 | DELTA3 | OLD4 | DELTA4 | OLD5 | DELTA5 | ITER | SUBIT | SSE |
|---|---|---|---|---|---|---|---|---|---|
| 1 | . | . | . | . | . | . | 0 | 0 | 182.175 |
| 2 | 21.5076 | -20.495 | 0.2355 | -0.2334 | 0.8668 | 1.5418 | 1 | 0 | 474.566 |
| 3 | 21.5076 | -10.247 | 0.2355 | -0.1167 | 0.8668 | 0.7709 | 1 | 1 | 110.838 |
| 4 | 11.2602 | -4.479 | 0.1188 | 0.0175 | 1.6377 | 0.6363 | 2 | 0 | 75.743 |
| 5 | 6.7815 | 0.546 | 0.1362 | -0.0063 | 2.2740 | 0.0480 | 3 | 0 | 72.668 |
| 6 | 7.3275 | 0.021 | 0.1300 | 0.0007 | 2.3219 | -0.0080 | 4 | 0 | 72.650 |
| 7 | 7.3489 | -0.002 | 0.1306 | -0.0000 | 2.3140 | 0.0014 | 5 | 0 | 72.650 |
| 8 | 7.3470 | -0.000 | 0.1306 | 0.0000 | 2.3153 | -0.0005 | 6 | 0 | 72.650 |

LIST DATA SET _VC

| OBS | ITER | U1 | U2 | U3 | LNLR | LASTLNLR | NOTES |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1.0000 | 1.00000 | 1.0000 | -522.78 | . | |
| 2 | 1 | 66.0858 | 9.84900 | 11.7697 | -192.10 | -522.78 | |
| 3 | 2 | 85.6661 | 0.89740 | 11.7920 | -191.07 | -192.10 | |
| 4 | 3 | 89.8449 | 0.47875 | 11.7793 | -191.05 | -191.07 | |
| 5 | 4 | 89.9844 | 0.51815 | 11.7707 | -191.05 | -191.05 | |
| 6 | 5 | 89.9860 | 0.51338 | 11.7717 | -191.05 | -191.05 | |

LIST DATA SET OUTDATA

| OBS | ALPHA | AM2 | AM3 | OMEGA | LAMBD | OLD1 | DELTA1 |
|---|---|---|---|---|---|---|---|
| 1 | 66.7874 | 5.80879 | 7.34686 | 0.130643 | 2.3148 | 66.7854 | 0.00205844 |
| 2 | 66.7874 | 5.80879 | 7.34686 | 0.130643 | 2.3148 | 66.7854 | 0.00205844 |
| 3 | 66.7874 | 5.80879 | 7.34686 | 0.130643 | 2.3148 | 66.7854 | 0.00205844 |
| ⋮ | | | | | | | |
| 69 | 66.7874 | 5.80879 | 7.34686 | 0.130643 | 2.3148 | 66.7854 | 0.00205844 |

| OBS | OLD2 | DELTA2 | OLD3 | DELTA3 | OLD4 | DELTA4 |
|---|---|---|---|---|---|---|
| 1 | 5.80883 | -0.000039929 | 7.347 | -0.00013741 | 0.130629 | 0.0000137185 |
| 2 | 5.80883 | -0.000039929 | 7.347 | -0.00013741 | 0.130629 | 0.0000137185 |
| 3 | 5.80883 | -0.000039929 | 7.347 | -0.00013741 | 0.130629 | 0.0000137185 |
| ⋮ | | | | | | |
| 69 | 5.80883 | -0.000039929 | 7.347 | -0.00013741 | 0.130629 | 0.0000137185 |

| OBS | OLD5 | DELTA5 | ITER | SUBIT | MOIST | X | Y | YEAR | BLK | MDUM (1 | MDUM 2 | MDUM 3) | E |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.31533 | -0.00053346 | 6 | 0 | + | 0.054 | 60.0833 | 2 | 1 | 0 | 1 | 0 | 0.878649 |
| 2 | 2.31533 | -0.00053346 | 6 | 0 | + | 0.065 | 56.6701 | 2 | 1 | 0 | 1 | 0 | 0.819788 |
| 3 | 2.31533 | -0.00053346 | 6 | 0 | + | 0.081 | 50.5791 | 2 | 1 | 0 | 1 | 0 | 0.718414 |
| ⋮ | | | | | | | | | | | | | |
| 69 | 2.31533 | -0.00053346 | 6 | 0 | T | 0.088 | 67.3976 | 6 | 1 | 0 | 0 | 1 | 0.669879 |

| OBS | F | DERALPHA | DERAM2 | DERAM3 | DER OMEGA | DER LAMBDA | YHAT | RESID |
|---|---|---|---|---|---|---|---|---|
| 1 | 63.7866 | 0.878649 | 0.878649 | 0 | 146.214 | 7.29054 | 63.7866 | -3.703 |
| 2 | 59.5135 | 0.819788 | 0.819788 | 0 | 209.537 | 8.25542 | 59.5135 | -2.843 |
| 3 | 52.1541 | 0.718414 | 0.718414 | 0 | 305.607 | 8.24479 | 52.1541 | -1.575 |
| ⋮ | | | | | | | | |
| 69 | 49.6610 | 0.669879 | 0 | 0.669879 | 352.547 | 7.86194 | 49.6610 | 17.7366 |

LIST DATA SET NEQ

| OBS | XVIX_001 | XVIX_002 | XVIX_003 | XVIX_004 | XVIX_005 | XVIY |
|---|---|---|---|---|---|---|
| 1 | 0.072 | 0.046 | 0.0106 | -46.1 | -0.92 | -0.0000 |
| 2 | 0.046 | 0.827 | -0.2062 | -23.1 | -0.39 | -0.0000 |
| 3 | 0.011 | -0.206 | 0.4211 | -3.9 | -0.09 | 0.0000 |
| 4 | -46.066 | -23.103 | -3.9330 | 54619.9 | 1244.10 | 0.0104 |
| 5 | -0.922 | -0.385 | -0.0949 | 1244.1 | 35.36 | 0.0015 |
| 6 | 59.41 | 32.843 | 8.4989 | 10771.4 | 431.15 | 72.6495 |

LIST DATA SET VEQ

| OBS | MLEQ_01 | MLEQ_02 | MLEQ_03 | YQVQY | CMP_NAME |
|---|---|---|---|---|---|
| 1 | 3.63274E-04 | 2.42211E-04 | 1.68657E-05 | 3.30126E-02 | SIGMA_01 |
| 2 | 2.42211E-04 | 6.76251E-01 | 6.85245E-02 | 1.17600E+00 | SIGMA_02 |
| 3 | 1.68657E-05 | 6.85245E-02 | 4.69019E-01 | 5.55785E+00 | ERROR |
| 4 | 8.99860E+01 | 5.13381E-01 | 1.17717E+01 | -1.91046E+02 | PRIORS |
| 5 | 3.00000E+00 | 5.00000E+00 | 6.90000E+01 | . | LEVELS |

LIST DATA SET _VEQMML

| OBS | QVQV_01 | QVQV_02 | QVQV_03 | YQVQY | CMP_NAME |
|---|---|---|---|---|---|
| 1 | 2.41313E-04 | 1.60921E-04 | 2.74879E-05 | 3.30126E-02 | SIGMA_01 |
| 2 | 1.60921E-04 | 6.73475E-01 | 6.84576E-02 | 1.17600E+00 | SIGMA_02 |
| 3 | 2.74879E-05 | 6.84576E-02 | 4.39967E-01 | 5.55785E+00 | ERROR |
| 4 | 8.99860E+01 | 5.13381E-01 | 1.17717E+01 | -1.88879E+02 | PRIORS |
| 5 | 3.00000E+00 | 5.00000E+00 | 6.90000E+01 | . | LEVELS |