

Generalized Least Squares Estimation in Heteroscedastic Linear Models

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Introduction

In toxicology studies, increasing dose levels can often cause the animals to respond with greater variability to treatment. A new technique, introduced by Lin and Vonesh (1989), can be used to correct for inhomogeneity of variance. The Lin-Vonesh (LV) technique can also be used to correct for non-normality and outliers.

This paper will describe:

- How to compute the LV estimator for ANOVA models using PROC NLIN in SAS*.
- Limited Monte Carlo studies that evaluate the estimator's performance under heteroscedasticity and in the presence of outliers.
- Techniques for identifying outliers, inhomogeneity, and nonlinearity.
- The use of general transformations to normality.
- Methods for handling more complicated models.

In the limited simulation studies described here, the LV estimator performed well against the naive application of Ordinary Least Squares (OLS) and is worthy of further investigation.

The Lin-Vonesh Estimator

Tests comparing treatment and control can conveniently be expressed as a General Linear Model:

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + e_i, \quad e \sim F(0, \sigma)$$

where a dependent variable, y , is a function of a vector of independent variables, $\mathbf{x}$; a vector of unknown coefficients, $\boldsymbol{\beta}$; an unknown error term, e ; a common measure of scale, σ ; and an unspecified distribution function F . If σ is brought into the estimation equation and allowed to vary across the sample, and if a transformation is applied to the dependent variables to ensure normality, a Generalized Least Squares (GLS) estimator is created:

$$\sigma_i^{-1} g(y_i; \theta) = \sigma_i^{-1} \mathbf{x}_i' \boldsymbol{\beta} + \sigma_i^{-1} e_i, \quad \sigma_i^{-1} e_i \sim N(0, 1)$$

The errors are now normally distributed with mean zero and unit variance. The GLS estimator is inherently

nonlinear, requiring iterative estimation of σ and any parameters, θ , of the transformation $g(y; \theta)$.

Lin and Vonesh (1989) have suggested that if the residuals are assumed to be normally distributed and monotonically related to the ranks, r_i , of y_i , then e could be replaced by the BLOM scores (Blom, 1958 and Tukey, 1962) defined as:

$$z_i = \Phi^{-1}[(r_i - 3/8)/(n + 1/4)]$$

where Φ is the normal distribution. The residuals can then be shifted to the left-hand side of the equation:

$$z_i = \sigma_i^{-1} (y_i - \mathbf{x}_i' \boldsymbol{\beta}) = \sigma_i^{-1} g(U_i; \theta) - \sigma_i^{-1} \mathbf{x}_i' \boldsymbol{\beta}$$

converting the unknown error term to a known quantity. The BLOM scores can be constructed *within groups* using:

```
proc rank data = a normal = BLOM;
  by group; var y; ranks z;
```

The resulting estimates:

$$z_i = \sigma_i^{-1} e_i = \sigma_i^{-1} g(U_i; \theta) - \sigma_i^{-1} \mathbf{x}_i' \boldsymbol{\beta}, \quad z_i \sim N(0, 1)$$

will have minimum error subject to the constraint of normally distributed residuals.

It should be noted that: (i) the use of within-group BLOM scores does not solve the problem of inhomogeneous variances. Rather, it sets up the constraints necessary to simultaneously estimate all the parameters of the GLS model, and, (ii) a transformation, $g(U; \theta)$, of the order statistics (the sorted values of y or a function of them) might also be necessary to insure normality.

The estimator is still multiplicative and must be solved using nonlinear estimation in PROC NLIN, either through minimizing a likelihood equation:

$$\mathbf{u} = \mathbf{z} - \mathbf{F}(\boldsymbol{\beta}, \theta, \sigma) \\ L(\boldsymbol{\beta}, \theta, \sigma) = 0.5(\mathbf{u}' \mathbf{u})$$

or creating a gradient matrix:

$$\mathbf{X}'\mathbf{F}(\boldsymbol{\beta}, \boldsymbol{\theta}, \sigma) = \mathbf{X}'\mathbf{u}$$

$$\mathbf{X} = \frac{\partial \mathbf{F}}{\partial \boldsymbol{\beta}}$$

The normal equations can then be solved using an iterative Gauss-Newton algorithm. The derivatives for the linear ANOVA model and most commonly used transformations can be easily specified.

Single Sample

The LV estimator includes the additional step of replacing the residuals with BLOM scores. Because all GLS models approach the normal distribution in the limit, investigations which rely on asymptotic theory will not be very conclusive. The LV estimator can, alternatively, be studied using small-sample Monte Carlo techniques.

In the case of a single-sample with constant variance, the estimator of the overall mean, μ , is:

$$\sigma^{-1}(y_i - \mu) = \sigma^{-1}g(U_i; \theta) - \sigma^{-1}\mu$$

$$z_i = \Phi^{-1}[(r_i - 3/8)/(n+1/4)]$$

$$z_i = \sigma^{-1}g(U_i; \theta) - \sigma^{-1}\mu$$

When the y 's are normally distributed and do not require transformation, the derivatives of z with respect to each parameter are:

$$\frac{\partial z}{\partial \sigma} = -\frac{(y - \mu)}{\sigma^2}$$

$$\frac{\partial z}{\partial \mu} = -\frac{1}{\sigma}$$

The model and derivatives translate directly to PROC NLIN code in SAS:

```
proc nlin data=b nohalve;
  parms sigma=1 mu=1 ;
  model ry = (y - mu)/sigma;
  der.sigma = -(y - mu)/sigma**2;
  der.mu = -1/sigma;
```

The derivatives with respect to σ , for example, can be calculated directly in *Mathematica* (Wolfram, 1988) using:

```
D[(y - mu)/sigma, sigma]
```

or in *JMP** for the Apple Macintosh as part of the nonlinear data-fitting platform.

Monte Carlo experiments can then be run with the following SAS code:

```
%let sigma = 250; %let mu = 850;
%let n = 50; %let ng = 1;
do i = 1 to &ng;
  do j = 1 to &n;
    c = 1;
    y = &mu + &sigma*rannor(0);
    output;
  end;
end;
```

The parameter values for μ and σ were chosen to simulate platelet counts, a clinical chemistry parameter measured as $n/\mu\text{L}$, which is often poorly distributed with outliers.

The results of the estimation are presented in Appendix 1. Notice that the standard error of the mean is 37.66 in the OLS analysis and 5.37 in GLS. Which one is correct? The variance for any linear combination:

$$a = a_1Y_1 + a_2Y_2 + \dots + a_nY_n$$

is given by (Draper and Smith, 1981):

$$V(a) = a_1^2 V(Y_1) + a_2^2 V(Y_2) + \dots + a_n^2 V(Y_n)$$

If homoscedasticity is assumed, the variance can be written as:

$$V(a) = (a_1^2 + a_2^2 + \dots + a_n^2)\sigma^2$$

$$= \left(\sum a_i^2\right)\sigma^2$$

In the single sample model, each a is 1 and the sum-of-squares is n . Therefore, the standard error in the single sample model is:

$$se(\beta) = \frac{\sigma}{\sqrt{n}}$$

With $n=50$ and $\sigma=250$ in the simulation, $se(\beta)=35.36$, which is closer to the OLS result. The GLS standard errors are computed from the gradient rather than the design matrix using:

$$V(\beta) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

Evidently, the LV standard errors must then be computed manually.

To complete the Monte Carlo experiments, a large number of samples should be drawn. In each of the

experiments, 500 Monte Carlo replications for both OLS and GLS at $N=\{10, 20, 50, 100\}$ were drawn. The resulting parameter estimates for β (and σ) were then averaged using PROC MEANS and compared by constructing:

$$\text{Relative Bias} = \frac{|E(\beta_{OLS}) - \beta_{OLS}|}{|E(\beta_{GLS}) - \beta_{GLS}|}$$

$$\text{ARE} = \frac{V(\beta_{OLS})}{V(\beta_{GLS})}$$

measures of Bias and Asymptotic Relative Efficiency. The results, presented in Table I,

N	Bias		ARE	
	μ	σ	μ	σ
10	1.00	0.50	0.96	0.86
20	1.00	0.20	1.00	0.94
50	1.00	0.33	0.96	0.98
100	1.00	0.33	1.02	0.97

Table I. Single-sample

indicate favorable performance, except for the estimate of σ (values > 1.0 favor the LV estimator). In other words, if the data were truly drawn from a single-sample normal distribution, there would be little benefit in choosing the LV estimator. The relative bias measures for σ would not have produced different conclusions in, say, t -statistics because the absolute differences were small.

Analysis of Variance

In the case of a general linear model where all the values in X are indicator variables $[0,1]$, the LV ANOVA model becomes:

$$\sigma^{-1}(y_i - x_i'\beta) = \sigma^{-1}g(U_i) - \sigma^{-1}x_i'\beta$$

$$z_i = \sigma^{-1}g(U_i) - \sigma^{-1}x_i'\beta$$

with derivatives:

$$\frac{\partial z}{\partial \sigma} = -\frac{(y - \alpha - x\beta)}{\sigma^2}$$

$$\frac{\partial z}{\partial \alpha} = -\frac{1}{\sigma}$$

$$\frac{\partial z}{\partial \beta} = -\frac{x}{\sigma}$$

For a two-group experiment, the Monte Carlo sample can be drawn using:

```
%let n = 50; %let ng = 2;
do group = 1 to &ng;
  do j = 1 to &n;
    c = 1;
    y = &mu + (group-1)*&sigma +
        &sigma*rannor(0);
    x = (group=2) ;
    output;
  end;
end;
```

The results from these experiments, presented in Table II,

N	Bias			ARE		
	α	σ	β	α	σ	β
10	1.00	0.12	1.00	1.00	0.87	0.98
20	1.00	0.12	1.00	1.13	0.89	1.07
50	1.00	0.12	1.00	1.06	0.94	1.01
100	1.00	0.25	1.00	1.07	0.98	1.07

Table II. ANOVA

are similar to the single-sample runs. While the relative bias in σ appears to strongly favor the OLS estimator, the absolute values are small in magnitude and would not have changed the results of hypothesis testing.

Heterogeneous Variance

The Monte Carlo results to this point indicate there would be little advantage to using the LV estimator on data that meets OLS assumptions. This is as expected because the Gauss-Markov theorem (Wonnacott and Wonnacott, 1970: 21) shows that OLS is the Best Linear Unbiased Estimator (BLUE). That is, OLS has minimum variance when all assumptions are met.

In the heterogeneous variance case, however, the generalized Gauss-Markov theorem can also be used to show that OLS is biased (Wonnacott and Wonnacott, 1970: Chapter 16). To allow a different variance for each group, the LV estimator can be expanded:

$$\frac{(y_i - x_i'\beta)}{\sigma x_i'} = \frac{g(U_i) - (x_i'\beta)}{\sigma x_i'}$$

by introducing $(\sigma x')$, a vector of variances for each column of the design matrix. In the two group case, the derivatives are:

$$\frac{\partial z}{\partial \sigma_1} = -\frac{(y - \alpha - x\beta)}{(\sigma_1 + \sigma_2 x)^2}$$

$$\frac{\partial z}{\partial \sigma_2} = -\frac{x(y - \alpha - x\beta)}{(\sigma_1 + \sigma_2 x)^2}$$

$$\frac{\partial z}{\partial \alpha} = -\frac{1}{(\sigma_1 + \sigma_2 x)}$$

$$\frac{\partial z}{\partial \beta} = -\frac{x}{(\sigma_1 + \sigma_2 x)}$$

with σ_1 introduced for the constant term and σ_2 for the treatment effect. In the Monte Carlo simulation:

```
%let n = 50; %let ng = 2;
do group = 1 to &ng;
  do j = 1 to &n; c = 1;
    y = &mu + (group-1)*&sigma +
      &group*sigma*rannor(0);
    x = (group=2) ;
    output; end; end;
```

the variance has been doubled in the treatment group.

Note that initial Monte Carlo experiments with contrast coding [-1,1] for group comparisons (Freund, 1989) using:

```
x = (group=2) - (group=1);
```

produced unstable estimates in the LV model. Evidently, the computation of the derivative can become unstable when the design matrix is based on subtractions.

The Monte Carlo results, displayed in Table III,

N	Bias			ARE		
	α	σ	β	α	σ	β
10	1.00	7.05	1.00	0.99	1.14	1.05
20	1.00	15.67	2.00	0.91	1.19	0.99
50	1.00	24.00	0.29	0.94	1.39	0.98
100	1.00	24.00	0.75	0.98	1.26	1.03

Table III. Heteroscedasticity

indicate a superiority for the LV estimator, particularly with respect to the values of $\sigma=\sigma_1$ reported in the table.

Outliers

Another well-known violation of OLS assumptions involves the presence of outliers, which can be observations drawn from a different distribution. In toxicology studies, outliers often result from

measurement error or from unusual individual differences between animals.

In clinical chemistry measurements of platelet counts, individual values have been observed that would suggest the following single-sample Monte Carlo simulation:

```
%let n = 50; do j = 1 to &n-2;
  c = 1;
  y = &mu + &sigma*rannor(0);
  x = 0 ;
  output;
end;
x=1; group=2;
y = &mu - 750 + 3 * &sigma * rannor(0);
output;
y = &mu - 750 + 3 * &sigma * rannor(0);
output;
```

where two animals per group would have unusually low counts. Notice that the outliers have been identified *as if they were another group*, allowing the LV heterogeneous ANOVA estimator to be used.

N	Bias			ARE		
	α	σ	β	α	σ	β
10	1.76	2.73		1.17	1.70	
20	2.12	2.72		1.28	2.05	
50	1.93	3.05		1.13	1.97	
100	1.50	2.85		1.06	1.95	
10	0.04	0.89	0.04	0.77	1.15	0.67
20	0.03	0.72	0.00	1.05	1.24	0.45
50	0.07	0.77	1.43	1.02	1.32	0.32
100	0.10	0.77	0.30	0.99	1.13	0.30

Table IV. Outliers

The LV estimator was compared against both a naive OLS estimate (top panel in Table IV) and against an OLS estimator where the outliers were identified in the design matrix (but where a single variance was assumed). The results indicate better ARE for σ , but not necessarily better for other parameters in the model.

In other words, using the LV model only to estimate the variance of a few outlying observations may not be worth the effort.

Testing Assumptions

The Monte Carlo results indicate that the LV estimator should *not* be routinely used unless departures from OLS assumptions can be demonstrated. Some approaches to testing assumptions are:

Outlier Identification. The use of *Influence Analysis* involves determining the effect each observation has on model parameters. The *hat matrix*:

$$h_i = \mathbf{x}_i(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_i$$

is computed by dropping the *i*-th row of the design matrix and recomputing the parameter estimate.

Belsely, Kuh, and Welsch (1980) recommend a cutoff value for *h* of $(2p)/n$ where *p* is the number of parameters in the model. The INFLUENCE option in PROC REG produces an output data set with *h* values.

Testing Homogeneity of Variance. A test developed by Levene (1960) and generalized by Draper and Hunter (1969) can be constructed using the absolute values of the regression residuals to test for homogeneity of variance.

Testing for Normality. A test developed by Shapiro and Wilk (1965) can be applied to the residuals using PROC UNIVARIATE.

These considerations suggest that, prior to using the LV estimator, the OLS assumptions should be tested using:

```
proc reg data = a;
  model y = x1 x2 x3 / influence;
  output out = r r = resid dfits = yd;
data r;
  set r;
  x4 = (yd > 2*sqrt(sp / sn));
  resid = abs(resid);
proc reg data = r;
  title "Levene Test";
  model resid = x1 x2 x3 x4;
proc univariate data = r plot normal;
  var resid;
```

If the assumptions have not been violated, the OLS estimates remain BLUE.

Weighting

The approach taken above to identifying outliers and heterogeneous variances is not the only way the LV model can be used. A weighting function (Nelder and Wedderburn, 1972; Draper and Smith, 1981; Carroll and Ruppert, 1988) can be constructed:

$$\mu_x = f(X)$$

$$\text{var}(Y) = \sigma_y^2 = \sigma_x^2 [f'(\mu_x)]^2$$

to down-weight outliers or provide continuous adjustment to variances in covariance or regression analysis. The LV model then becomes:

$$\sigma_i^{-1} \omega_i^{-1} g(y_i; \theta) = \sigma_i^{-1} \omega_i^{-1} \mathbf{x}_i' \beta + \sigma_i^{-1} \omega_i^{-1} e_i$$

$$\sigma_i^{-1} \omega_i^{-1} e_i \sim N(0,1)$$

Notice that the spirit of the GLS estimator is to include the estimation of the variance parameter as a part of the regression problem.

Weighting functions have also been suggested for correcting heteroscedasticity or down-weighting outliers. Among them, the Tukey bi-weight estimator (Beaton and Tukey, 1974) and the use of rank-based weighting (Hettmansperger and McKean, 1977) have all been suggested as possibilities. The `_WEIGHT_` variable in PROC NLIN could then be used with the LV estimator in SAS.

Transformations

Transformations have also been routinely used to correct for both non-normality and heteroscedasticity.

- **Arithmetic transformations.** Draper and Hunter (1969) have suggested using a series of transformations (e.g., log, square root, arcsin, etc.) until either the normal-theory assumptions have been met or the procedure fails. The Box-Cox or generalized log transformation (Box and Cox, 1964) has been widely used for continuous data:

$$g(y, \lambda, c) = \frac{(y+c)^\lambda - 1}{\lambda} \quad \text{if } \lambda \neq 0$$

$$= \ln(y+c) \quad \text{if } \lambda = 0.$$

For categorical data, there have been a number of suggested transformations. Mosteller and Tukey (1977) have suggested the generalized logit:

$$g(y, \lambda) = \frac{y^\lambda - (1-y)}{\lambda} \quad \text{if } \lambda \neq 0$$

$$= \ln[y/(1-y)] \quad \text{if } \lambda = 0.$$

Guerrero and Johnson (1982) have suggested another form of the generalized logit:

$$g(y, \lambda) = \frac{[y/(1-y)]^\lambda - 1}{\lambda} \quad \text{if } \lambda \neq 0$$

$$= \ln[y/(1-y)] \quad \text{if } \lambda = 0.$$

as has Aranda-Ordaz (1981):

$$g(y, \lambda) = \frac{[y/(1-y)]^\lambda - 1}{\lambda[y/(1-y)]^\lambda + 1} \quad \text{if } \lambda \neq 0$$

$$= \ln[y/(1-y)] \quad \text{if } \lambda = 0.$$

In practice, the search for an appropriate transformation can be time consuming and can fail either due to the shape of the underlying distribution or to the presence of outliers (Thakur, Trutter, and Korte, 1983). Even if a transformation can be found, it might not have a scientifically acceptable explanation.

- **Rank transformations (RT).** The RT approach has become popular based on the work of Conover and Iman (1981). Carrying out an RT procedure involves replacing the original observations by the ranks and then calculating the usual parametric statistics.

The rank model can be fit more generally within the GLS framework by using the Beta family of transformations (Rocke, 1993):

$$g_B(x; \lambda) = \int_0^x t^{\lambda-1} (1-t)^{\lambda-1} dt$$

Where $\lambda=0$ corresponds to the logit transformation, $\lambda=.5$ corresponds to the arcsin square-root transformation, and $\lambda=1$ corresponds to a uniform distribution (Johnson and Kotz, 1970).

More Complicated Models

In models that go beyond one-way ANOVA, there are a number of other issues that must be studied:

- BLOM scores must be calculated within each *cross-classified* group in the design.
- The meaning of interaction terms in the transformed scale may no longer be clear (Sampson and Guttorp, 1991).

These, and other issues, could be studied by the same techniques presented above.

Discussion

In this article, a GLS estimator suggested by Lin and Vonesh (1989) was investigated using limited Monte Carlo sampling.

The first set of simulations involved conditions where a GLS estimator was really not needed, i.e., single- and multiple-sample data drawn from a normal distribution with homogeneous errors. As would be expected from the Gauss-Markov theorem, OLS has higher ARE, but not dramatically so.

In the case of heterogeneous variances, ARE is higher for the GLS estimator but only for the estimate of σ . The group means were estimated with essentially equal efficiency by OLS.

In the presence of outliers, the GLS estimator produced less biased estimates of σ but did worse than OLS in estimating the magnitude of the outlier effect.

These results suggest that the Lin-Vonesh technique would be useful in situations where variances across groups are not equal. What remains to be investigated is its performance under conditions of non-normality and against other GLS-class estimators and nonparametric methods.

Programming the Lin-Vonesh technique in SAS has some drawbacks, including computation of derivatives, calculation of standard errors by hand, and the inability to use contrast coding. Each of these difficulties could be corrected by writing custom software.

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Appendix 1. Estimation Results.

ANOVA Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
C	1	907.502981	37.65720989	24.099	0.0001

GLS Parameter Estimates

Parameter	Estimate	Asymptotic Std. Error	Asymptotic 95 % Confidence Interval	
			Lower	Upper
SIGMA	276.1292954	5.5848932751	264.90014242	287.35844841
MU	875.3303350	5.3739119594	864.52538732	886.13528265