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On Drawbacks of Least Squares Lehmann-Scheffé Estimation of Variance Components

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Abstract

Estimation of variance components is one of the basic problems in linear models with mixed effects, and a vast literature exists on the subject. Unfortunately, there are only few situations in which uniformly best estimators exist, which usually results into need of using an iterative estimation procedure. A new non-iterative method, called Least Squares Lehmann-Scheffé method, was proposed and its superiority over commonly accepted methods was claimed. We show that the situation is not that simple.

Keywords: least squares estimation, mixed linear model, variance components.

1 Introduction

Estimation of variance components is one of the basic problems in linear models with mixed effects, and a vast literature exists on the subject. Two major problems appear in practical applications:

1. the uniformly best unbiased estimators, which do not depend on values of estimated parameters, exist only in very special cases;

2. majority of estimation methods are iterative.

If we are not lucky enough to have a very nice design, then we have two options: either to use a general method of estimation such as Henderson method 3, ML, REML, or to use some locally best estimators. In most of

them, however, we have to choose some starting (prior) values of estimated parameters and/or go through an iterative estimation procedure.

Slanger (1996) introduced a new method of estimation of variance components, which eliminates both problems: no prior values of parameters are needed and the method is non-iterative. It can be applied in any linear model with mixed effects. According to the author, it is based on the Lehmann-Scheffé theorem. Since it uses least-squares principle, the proposed method is called the least-squares Lehmann-Scheffé method (LSLS method).

Slanger (1996) also compared his method with Henderson method 3 in one simple model, and Slanger & Carlson (2003) compared the method with REML in six simulated designs. Superiority of the new method was claimed in all cases. However, as we are going to show, there are serious concerns about mathematical properties of the LSLS method.

2 Principle of the method

Mixed linear model in its simplest form can be written as

$$Y = X\beta + Z\alpha + \varepsilon, \tag{1}$$

where X and Z are known design matrices, β are fixed effects, and α random effects. If the covariance structure is supposed to be $\mathrm{var}(\varepsilon) = \sigma_\varepsilon^2 I$ and $\mathrm{var}(\alpha) = \sigma_\alpha^2 A$, we have

$$\begin{aligned} \mathrm{E}(Y) &= X\beta, \\ \mathrm{var}(Y) &= \sigma_\alpha^2 ZAZ' + \sigma_\varepsilon^2 I \stackrel{\mathrm{df}}{=} \sigma_\alpha^2 J + \sigma_\varepsilon^2 I. \end{aligned} \tag{2}$$

Let P_X and $M_X = I - P_X$ be the matrices of orthogonal projection onto the subspace generated by the columns of matrix X and onto its orthogonal complement, respectively. Slanger (1996) proposed to estimate the variance components by functions

$$\widehat{\sigma}_\varepsilon^2 = Y' M_X Q_\varepsilon M_X Y \quad \text{and} \quad \widehat{\sigma}_\alpha^2 = Y' M_X Q_\alpha M_X Y\,. \tag{3}$$

Since

$$\begin{aligned} \mathrm{E}(Y' M_X Q M_X Y) &= \mathrm{Tr}\left[Q M_X \,\mathrm{var}(Y) M_X\right] = \\ &= \sigma_\alpha^2 \left[\mathrm{vec}(M_X J M_X)\right]' \mathrm{vec}(Q) + \sigma_\varepsilon^2 \left[\mathrm{vec}(M_X)\right]' \mathrm{vec}(Q) \end{aligned} \tag{4}$$

(the vec() operator working column-wise), unbiased estimating matrices Q_ε and Q_α must fulfill

$$\left[\mathrm{vec}(M_X)\right]' \mathrm{vec}(Q_\varepsilon) = 1 \quad \text{and} \quad \left[\mathrm{vec}(M_X J M_X)\right]' \mathrm{vec}(Q_\varepsilon) = 0,$$

$$[\mathrm{vec}(M_X)]' \mathrm{vec}(Q_\alpha) = 0 \quad \text{and} \quad [\mathrm{vec}(M_X J M_X)]' \mathrm{vec}(Q_\alpha) = 1.$$

According to Lehmann-Scheffé theorem (see Lehmann & Scheffé (1950)), unbiased estimator T of some statistic $h(\theta)$ is uniformly minimum variance unbiased estimator (UMVUE) in a class $\mathcal{T}$, if it is uncorrelated with every statistic $Z \in \mathcal{T}$ with zero mean value and finite variance. The author considered only statistics Z of the form $Y'M_XSM_XY$, where S is some appropriate matrix. Because of zero mean value, matrix S must fulfill

$$\begin{pmatrix} [\mathrm{vec}(M_X)]' \\ [\mathrm{vec}(M_X J M_X)]' \end{pmatrix} \mathrm{vec}(S) \stackrel{\mathrm{df}}{=} B \,\mathrm{vec}(S) = 0, \tag{5}$$

i. e., $\mathrm{vec}(S)$ must lie in the nullspace of B. Let $\mathrm{vec}(C_1), \ldots, \mathrm{vec}(C_m)$ be a basis of this nullspace, then $S = \sum_{i=1}^{m} k_i C_i$, where k_i are some real numbers. Under normality assumption, the covariance between $Y'M_XQM_XY$ and $Y'M_XSM_XY$ is

$$\begin{aligned} \mathrm{cov}(Y'M_XQM_XY, Y'M_XSM_XY) = \\ = 2\sigma_\alpha^4 [\mathrm{vec}(M_X J M_X S M_X J M_X)]' \mathrm{vec}(Q) + \\ + 2\sigma_\alpha^2 \sigma_\varepsilon^2 [\mathrm{vec}(M_X J M_X S M_X + M_X S M_X J M_X)]' \mathrm{vec}(Q) + \\ + 2\sigma_\varepsilon^4 [\mathrm{vec}(M_X S M_X)]' \mathrm{vec}(Q). \end{aligned}$$

Then, LSLS-estimator is uncorrelated with all statistics Z if it holds $\forall\, i$

$$\begin{gathered} [\mathrm{vec}(M_X J M_X C_i M_X J M_X)]' \mathrm{vec}(Q) = 0, \\ [\mathrm{vec}(M_X J M_X C_i M_X + M_X C_i M_X J M_X)]' \mathrm{vec}(Q) = 0, \\ [\mathrm{vec}(M_X C_i M_X)]' \mathrm{vec}(Q) = 0. \end{gathered} \tag{6}$$

If we denote $C_v = (\mathrm{vec}(C_1), \ldots, \mathrm{vec}(C_m))$, then equations (6) can be rewritten in the form

$$\begin{pmatrix} C_v'(M_X J M_X \otimes M_X J M_X) \\ C_v'(M_X J M_X \otimes M_X + M_X \otimes M_X J M_X) \\ C_v'(M_X \otimes M_X) \end{pmatrix} \mathrm{vec}(Q) \stackrel{\mathrm{df}}{=} R_0 \,\mathrm{vec}(Q) = 0,$$

where $\otimes$ is the Kronecker product. Let e_i denote the vector of appropriate dimension containing 1 at i-th place and zeros otherwise. Negative i denotes position counted from the end (-1 being the last position). Thus, LSLS-estimator must satisfy

$$\begin{pmatrix} B \\ R_0 \end{pmatrix} \mathrm{vec}(Q) \stackrel{\mathrm{df}}{=} R \,\mathrm{vec}(Q) = h, \tag{7}$$

where $h = e_2$ for Q_α, and $h = e_1$ for Q_ε. A least-squares solution is

$$\mathrm{vec}(\hat{Q}) = (R\,'R)^{-}R\,'h.$$

If $R\,\mathrm{vec}(\hat{Q}) - h = 0$, UMVUE is claimed to be found. If $R\,\mathrm{vec}(\hat{Q}) - h \neq 0$, MP-inverse for $\mathrm{vec}(\hat{Q})$ is used. This solution is called LSLS-estimator in both cases (also denoted by LSLS_b because of possible bias). LSLS-estimator is claimed to be the estimator which is as close as analytically possible to satisfying the Lehmann-Scheffé criterion.

Because exact solution of system (7) exists only in special cases, the author proposed to use Lagrange multipliers method to assure unbiasedness of the estimator together with almost zero covariance property. This estimator, denoted by LSLS_u, is the solution of system

$$\begin{pmatrix} R_0'R_0 & B' \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathrm{vec}(Q) \\ \lambda \end{pmatrix} = h,$$

where $h = e_{-1}$ for Q_α and $h = e_{-2}$ for Q_ε.

Generalization of the method to more variance components is simple. Every row of the matrix B in (5) must correspond to one variance component, there will be more restrictions to zero covariance in (6), and more right-hand-side vectors $h = e_i$ have to be used.

3 Analysis of the method

Although promised features of the method seem to be nice, and simulations done by the author look like confirming it, the reality is rather different. The method has some serious drawbacks, which will be analyzed in detail. Main problems are:

1. no reasonable properties of the estimators are assured;

2. mean value of an estimator can be a function of true values of all variance components;

3. the method tries to provide uniformly best estimators even if they do not exist;

4. the estimators are not unique.

Optimality properties of LSLS estimators

Author's hope for the good/optimality properties of the estimators are based on Lehmann-Scheffé theorem. It is true, that it suffices to consider quadratic estimators in the case of normally distributed vector of observations Y. However, the theorem guarantees the optimality in the given family of estimators only in the case, when the assumptions are met (i.e. zero covariance with all estimators of zero), and does not say anything about the other cases. As a consequence, no optimality properties are guaranteed in the case when approximate data-driven solution ("almost zero covariance") is used. Metric in the space of distributions can be quite different than that in data space. This holds for both LSLS_b and LSLS_u estimators.

The author chose to use matrix M_X to transform the values of Y. In fact, such projection leads to translation-invariant estimators. But this choice of the projector does not take into consideration the information about covariance between the elements of Y. If we want invariance, it would be better to use $M_X^{V^{-1}} = I - X(X'V^{-1}X)^{-}X'V^{-1}$ with $V = \mathrm{var}(Y)$, instead. But to use that, we need to know prior values of estimated parameters (or their first stage estimates), and it was not wished. This is how the problem of prior values was avoided, but not solved.

However, there is another – and bigger – problem with this transformation. The method is not applicable in models, where invariant unbiased estimators of variance components do not exist. If we consider model (1) with mean and variance structure (2), general theory of variance components models (see e.g. Rao & Kleffe (1980)) says that function $\gamma = f_1'\sigma_\alpha^2 + f_2'\sigma_\epsilon^2$ is unbiasedly estimable if and only if $f = (f_1, f_2)' \in \mathcal{R}(H)$, where

$$H = \begin{pmatrix} \mathrm{Tr}(J^2 - P_X J P_X J) & \mathrm{Tr}(M_X J) \\ \mathrm{Tr}(M_X J) & \mathrm{Tr}(M_X) \end{pmatrix},$$

and $\mathcal{R}(\cdot)$ denotes the range of a matrix. Function $\gamma = f'\theta$ is unbiasedly and invariantly (with respect to the mean shift) estimable if and only if $f \in \mathcal{R}(H_I)$, where

$$H_I = \begin{pmatrix} \mathrm{Tr}(M_X J) & \mathrm{Tr}(M_X J) \\ \mathrm{Tr}(M_X J) & \mathrm{Tr}(M_X) \end{pmatrix}.$$

Let us now consider the case, when a function γ is unbiasedly estimable, but not invariantly estimable, i. e. $f \in \mathcal{R}(H)$ & $f \notin \mathcal{R}(H_I)$.

Using LSLS method, variance components are estimated in the model

$$Y^* = M_X Z\alpha + \varepsilon^*,$$

where $Y^* = M_X Y$, and $\varepsilon^* = M_X \varepsilon$. In this model holds

$$\mathrm{E}(Y^*) = 0 \quad \text{and} \quad \mathrm{var}(Y^*) = \sigma_\alpha^2 M_X J M_X + \sigma_\varepsilon^2 M_X \,.$$

Function γ is unbiasedly estimable if and only if $f \in \mathcal{R}(H^*)$, where H^* is constructed as above. But in this model $X^* = 0$, so that $H^* = H_I$. Thus, no unbiased invariant estimator of γ exists, but LSLS-method still claims to provide such a one. The problem is that pre-multiplying of Y by M_X automatically eliminates all non-invariant estimators.

Example: Let us consider a model

$$Y_1 = \beta + \varepsilon_1,\ Y_2 = \beta + \varepsilon_2,$$

$$\mathrm{E}(\varepsilon_1^2) = \sigma_1^2,\ \mathrm{E}(\varepsilon_2^2) = \sigma_2^2,\ \mathrm{E}(\varepsilon_1 \varepsilon_2) = 0.$$

Then, using LSLS_u method, we obtain estimators $\hat{\sigma}_i^2 = Y' Q_{\sigma_i^2} Y$, $i = 1, 2$, where

$$Q_{\sigma_1^2} = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}, Q_{\sigma_2^2} = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}.$$

It means that $\hat{\sigma}_1^2 = \hat{\sigma}_2^2$, regardless of their true values.

Mean value of LSLS estimators

Since the system (7) need not be solved exactly and it holds (4), LSLS-estimator need not be unbiased. It means that the mean value of estimator is the linear combination of all variance components and the bias depends on the true values of all components. This can lead to severe bias, if the variance components differ substantially.

Uniform optimality property

As it was already stated, in most models there exist only locally best estimators, and uniformly best estimators do not exist. The method does not take into consideration such a fact and it tries to come as close as possible to such non-existing estimators. That is a very hard task. Thus, relationship to alternative estimators is unclear.

Uniqueness of LSLS estimators

The LSLS estimator is obtained by solving the system (7). This system is not solvable for unbalanced models, as the author stated. But there exist

also balanced models, for which the system (7) is not solvable. Example of such a model is the following one: $Y = X\beta + Z\alpha + \varepsilon$, where

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}', \; Z = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}'.$$

Therefore, the system can be "solved" in many cases only approximately. The following objections can be raised:

The author proposed the least-squares method, which leads to infinitely many Q matrices. One of the solutions is then chosen using Moore–Penrose g-inverse, which minimizes the Euclidean norm of the residual vector. This approach does not take into account variances of the observations; a variance-based norm could be more appropriate.

There is more to the last argument. Zero correlation estimators are denoted by T' and they are of the form $Y'M_XSM_XY$, where S is the matrix determined from (5). But such a matrix is not unique. Therefore, the basis of the nullspace of the matrix B is found in order to cover all suitable matrices S. The problem is, that there are infinitely many bases of the nullspace of matrix B and it is not clear, which basis should be chosen. For example let us consider model (1), where

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

and let $\mathrm{var}(\alpha) = \sigma_\alpha^2 I_3$ and $\mathrm{var}(\varepsilon) = \sigma_\varepsilon^2 I_4$. Now, let us consider two different bases of nullspace of matrix B

$$C_v^1 = \begin{pmatrix} -1 & 1 & 1 & -2 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & -4 & \frac{1}{2} & \frac{1}{2} & \frac{3}{2} & \frac{3}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

and

$$C_v^2 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & 2 & 1 & 0 & 0 & -1 & 1 \\ 0 & 0 & -3 & \frac{1}{2} & \frac{3}{2} & \frac{3}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Using them, we obtain LSLS_u estimators ${}_1\hat{\sigma}_\alpha^2$ and ${}_1\hat{\sigma}_\varepsilon^2$ or ${}_2\hat{\sigma}_\alpha^2$ and ${}_2\hat{\sigma}_\varepsilon^2$, where ${}_i\hat{\sigma}^2$ is LSLS_u estimator of variance component using basis C_v^i. Then, we get two different pairs of estimators, for which holds

$$\mathrm{var}({}_2\hat{\sigma}_\alpha^2) - \mathrm{var}({}_1\hat{\sigma}_\alpha^2) = 0.0028412\sigma_\alpha^4 + 0.0555613\sigma_\alpha^2\sigma_\varepsilon^2 + 0.056618\sigma_\varepsilon^4, \quad (8)$$

$$\mathrm{var}({}_2\hat{\sigma}_\varepsilon^2) - \mathrm{var}({}_1\hat{\sigma}_\varepsilon^2) = 0.0018456\sigma_\alpha^4 + 0.0172609\sigma_\alpha^2\sigma_\varepsilon^2 + 0.0202595\sigma_\varepsilon^4, \quad (9)$$

where σ_α^2 and σ_ε^2 are true parameter values. The differences (8) and (9) are always positive. As a result, the variance of the estimator obtained using basis C_v^2 is always greater than the variance of the estimator obtained using basis C_v^1. Such a dependence on the choice of the basis is very unfortunate.

Further, author suggested to reduce the number of equations in system (7). He suggested to use the vech operator in matrix B instead of vec operator. Vech operator makes a vector from any symmetric matrix stacking its columns one under another taking into consideration only elements on and under the diagonal. In such a way the number of columns in matrix B will reduce from original n^2 to $\frac{1}{2}n(n+1)$. The number of elements of basis of the nullspace of this matrix will reduce, too. But again, in the same model the vec-based estimators and vech-based estimators differ, and have different variances. It is not clear, which way gives estimators with smaller variance. There is no rule of thumb, since both can be better.

4 Simulations

We have conducted small simulation study to verify theoretical claims. We have considered two models:

- mixed effects two-way model (see Christensen (2011, Ex. 12.7))

$$y_{ijk} = \mu + \alpha_i + \eta_j + \gamma_{ij} + \varepsilon_{ijk}, \quad i = 1, 2,\ j = 1, 2, 3,\ k = 1, \ldots, n_{ij},$$

$n_{ij} \in \big[[3,5,5],[6,3,3]\big]$ with fixed α and random η and γ, and

- random effects model, all as before but with random α.

All random effects were simulated independent with normal distribution. 5,000 estimates of unknown parameters were computed using LSLS-method, LSLS_u-method, ML, REML, and Henderson method 3 in all cases.

Summarized results from the mixed effects model are in the following tables. Because of the problem with negative values acquired by some estimators, we give both overall sample means and sample means of positive values only.

method	Henderson 3	LSLS_b	LSLS_u	ML	REML
	$\sigma^2_\eta = 784$				
average	773.18	439.44	23.45	513.74	772.41
st. error	11.35	6.44	0.33	7.55	11.32
average of > 0	796.78	451.54	23.71	529.95	794.82
st. error of > 0	11.51	6.52	0.33	7.67	11.49
percentage of > 0	97.12%	97.40%	98.94%	96.94%	97.18%

method	Henderson 3	LSLS_b	LSLS_u	ML	REML
	$\sigma^2_\gamma = 25$				
average	25.47	21.65	52.40	15.52	28.11
st. error	0.60	0.52	0.72	0.35	0.55
average of > 0	42.85	36.81	59.11	28.25	42.03
st. error of > 0	0.73	0.63	0.73	0.52	0.71
percentage of > 0	67.02%	66.56%	89.88%	54.94%	66.88%

method	Henderson 3	LSLS_b	LSLS_u	ML	REML
	$\sigma^2_\epsilon = 64$				
average	64.15	64.06	63.48	61.86	62.95
st. error	0.29	0.29	0.29	0.29	0.28
average of > 0	64.15	64.06	63.48	61.86	62.95
st. dev. of > 0	0.29	0.29	0.29	0.29	0.28
percentage of > 0	100%	100%	100%	100%	100%

The same summary of the random effects model results is the following:

method	Henderson 3	LSLS_b	LSLS_u	ML	REML
	$\sigma^2_\alpha = 160$				
average	171.39	91.59	29.19	107.29	169.06
st. error	4.41	2.21	0.32	2.20	3.50
average of > 0	278.56	140.94	29.19	164.70	213.24
st. error of > 0	5.74	2.82	0.32	2.92	4.14
percentage of > 0	66.92%	69.00%	100%	65.14%	79.28%

method	Henderson 3	$LSLS_b$	$LSLS_u$	ML	REML
	$\sigma^2_\eta = 784$				
average	762.07	579.83	157.18	527.33	762.84
st. error	11.05	8.44	2.03	7.52	11.05
average of > 0	782.89	597.88	157.18	548.38	782.40
st. error of > 0	11.19	8.56	2.03	7.66	11.20
percentage of > 0	97.42%	97.06%	100%	96.16%	97.50%

method	Henderson 3	$LSLS_b$	$LSLS_u$	ML	REML
	$\sigma^2_\gamma = 25$				
average	25.82	46.07	141.77	31.02	25.94
st. error	0.61	0.59	1.53	0.61	0.52
average of > 0	42.64	49.65	141.77	44.30	38.96
st. error of > 0	0.74	0.60	1.53	0.77	0.67 2
percentage of > 0	67.80%	93.56%	100%	70.02%	66.60%

method	Henderson 3	$LSLS_b$	$LSLS_u$	ML	REML
	$\sigma^2_\epsilon = 64$				
average	64.13	64.61	173.01	63.07	62.89
st. error	0.29	0.29	1.65	0.29	0.28
average of > 0	64.13	64.61	173.01	63.07	62.89
st. error of > 0	0.29	0.29	1.65	0.29	0.28
percentage of > 0	100%	100%	100%	100%	100%

Our simulation did not confirm results of Slanger & Carlson (2003) that Slanger's method is superior to REML. According to our results, all methods have approximately the same precision for estimating σ^2_ε. $LSLS_u$ worked very badly in both models, estimates having hugely different values than those from the other methods (and the true parameter values). $LSLS_u$-estimates of σ^2_ε were heavily biased even in the random effects model. The only advantage of the method seemed to be lesser number of negative estimates when compared with the other methods. $LSLS_b$-method was very unreliable, sometimes giving reasonable values and sometimes fairly off.

5 Summary

Presented method has some advantages compared to widely used methods. It is not iterative and no prior values of unknown parameters are needed. But the method has also substantial drawbacks, which are the consequence of several theoretical mistakes. In fact, no optimality properties are assured, the estimators can be substantially biased, and they are not uniquely determined. Thus, estimators with quite different properties can be obtained from the same data. Moreover, our simulation results show that they are quite often severely biased. As a result, we cannot recommend this method for practical use.

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