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Estimation and incommutativity in mixed models

Dário Ferreira ^{a,*}, Sandra Ferreira ^a, Célia Nunes ^a, Miguel Fonseca ^b, Adilson Silva ^c, João T. Mexia ^b

^a Department of Mathematics and Center of Mathematics and Applications, Faculty of Sciences, University of Beira Interior, Covilhã, Portugal

^b Center for Mathematics and Applications, Faculty of Science and Technology, New University of Lisbon, Monte da Caparica, Portugal ^c Department of Mathematics, Faculty of Science and Technology, New University of Lisbon, Monte da Caparica, Portugal and Faculty of Science and Technology, University of Cape Verde, Cape Verde

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ABSTRACT

In this paper we present a treatment for the estimation of variance components and estimable vectors in linear mixed models in which the relation matrices may not commute. To overcome this difficulty, we partition the mixed model in sub-models using orthogonal matrices. In addition, we obtain confidence regions and derive tests of hypothesis for the variance components. A numerical example is included. There we illustrate the estimation of the variance components using our treatment and compare the obtained estimates with the ones obtained by the ANOVA method. Besides this, we also present the restricted and unrestricted maximum likelihood estimates.

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1. Introduction

There have been extensive studies of estimation in mixed models; see, e.g., [5,19,21–23]. In addition to a rich source of research publications, several books/monographs have been published in more recent years, such as [9,13,15]. Apart from that, the estimation of variance components in linear mixed models is not completely straightforward, even in the balanced case; see [6,14]. In what follows we will consider mixed models

$$Y = \sum_{i=0}^{w} X_i \beta_i, \tag{1}$$

where **Y** is a vector of *N* random variables $Y_1, ..., Y_N$, β_0 is a fixed vector and the $\beta_1, ..., \beta_w$ are random and independent vectors, with null mean vectors, variance–covariance matrices $V(\beta_i) = \theta_i I_{c_i}$ for all $i \in \{1, ..., w\}$, and null cross covariance matrices, $V(\beta_i; \beta_\ell) = \mathbf{0}_{c_i \times c_l}$ for all $i \neq \ell$. These models will have mean vector $\boldsymbol{\mu} = \mathbf{X}_0 \beta_0$ and variance covariance matrices

$$\boldsymbol{V}(\boldsymbol{Y}) = \sum_{i=1}^{w} \theta_i \boldsymbol{M}_i,$$

with $M_i = X_i X_i^{\top}$ for each $i \in \{1, ..., w\}$. So M_i is the $N \times N$ relation matrix for the sth random factor. That is, its (a, b)-entry is equal to 1 if this factor has the same level on units a and b, and otherwise it is equal to 0; see [2,3].

* Corresponding author.

E-mail address: dario@ubi.pt (D. Ferreira).

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In models in which the relation matrices M_1, \ldots, M_w commute, we have

$$\forall_{i\in\{1,\ldots,w\}} \quad \boldsymbol{M}_i = \sum_{j=1}^m b_{i,j} \boldsymbol{Q}_j,$$

where Q_1, \ldots, Q_m are known orthogonal symmetric idempotent matrices of order *N*, summing to the identity matrix I_N . Then the models have the variance covariance matrices

$$\boldsymbol{V}(\boldsymbol{\gamma}) = \sum_{j=1}^{m} \boldsymbol{\gamma}_{j} \boldsymbol{Q}_{j},$$

with $\gamma_j = \sum_{i=1}^{w} b_{i,j} \mathbf{Q}_i$ for all $j \in \{1, ..., m\}$. If the matrices $\mathbf{B} = [b_{i,j}]$ are invertible, the $\mathbf{V}(\boldsymbol{\gamma})$ will be the positive semi-definite linear combinations of $\mathbf{Q}_1, ..., \mathbf{Q}_m$ and the models will have orthogonal block structure (OBS, see [16,17]) which continue to play a very important role in the theory of randomized block designs; see [7,8]. Furthermore, there is a huge literature on mixed models and commutativity, starting with the work of [24,25]. Researchers like [1,18] also contributed to this area. A discussion of mixed models in which the relation matrices commute may be seen in [26]. A discussion on this assumption may also be found in [20,27]. Moreover, in [4] is investigated the case where the family of possible variance–covariance matrices, while still commutative, no longer forms an OBS.

The goal of this paper is to present a treatment of the estimation of variance components and estimable vectors in mixed models in which the relation matrices do not commute, or may not commute. To overcome this difficulty we partition the mixed model in sub-models using orthogonal matrices. Since V(Y) has an additive structure we say the models are additive, or ADD for short.

There are several popular methods available for the estimation of variance components in mixed models based on maximum likelihood, ML, or restricted maximum likelihood, REML. A review of this assumption may be seen in [11]. Analysis of variance, ANOVA, estimation based methods are also very popular. In particular, the three variations known as Henderson I, Henderson II, and Henderson III, suggested by [12]. Henderson I is the easiest to apply. Henderson II can be used for random models and Henderson III is the most suitable of the three methods.

The method we propose has some advantages over those mentioned above. We point out that our method can be applied without requiring normality or any other distribution for β_1, \ldots, β_w . So, unlike the ML, and REML estimators, it requires only that the distribution of β_1, \ldots, β_w has first and second moment. Besides this, our method is a unified method contrary to the ANOVA estimation based methods. That is, it can be applied to balanced or unbalanced, random or mixed models, whether or not the relation matrices commute.

In Section 2 we carry out estimation for variance components and estimable vectors in ADD models without requiring normality. We start with the algebraic structure of the models, from which we derive estimators for variance components. These estimators enable us to obtain generalized least squares, GLS, estimators for estimable vectors. In Section 3 we assume the model to be normal and use inducing pivot variables to obtain confidence intervals for the variance components; see [10]. These confidence intervals may be used, through duality, to test hypotheses about them. In Section 4 we present a numerical example in which we compare our technique for estimating variance components with unbalanced ANOVA. There we illustrate the estimation of the variance components using our treatment and compare the obtained estimates with the ones obtained by the ANOVA method. Besides this, we also present the REML and the ML estimated values. Finally we present some final comments in Section 5.

2. Additive models

2.1. Algebraic structure

We start by establishing the following result.

Proposition 1. Whatever the family $\underline{W} = \{W_1, \dots, W_w\}$ of symmetric $N \times N$ matrices, there exists an $N \times N$ matrix $P = [A_1^\top \cdots A_m^\top]^\top$ such that $A_j W_i A_j^\top = b_{i,j} I_{g_j}$ for all $i \in \{1, \dots, w\}$ and $j \in \{1, \dots, m\}$ with $g_j = \operatorname{rank}(A_j) = \operatorname{rank}(Q_j)$, where $Q_j = A_i^\top A_j$ for all $j \in \{1, \dots, m\}$.

Proof. We will use induction on w to establish the claim. The result is obviously true for w = 1, so let us assume that it is true for $w = \ell$. Then there will be an orthogonal matrix $\mathbf{P}_{\ell} = [\mathbf{A}_1^{\top}(\ell) \cdots \mathbf{A}_m^{\top}(\ell)]^{\top}$ such that $\mathbf{A}_j(\ell)\mathbf{W}_i\mathbf{A}_j^{\top}(\ell) = b_{i,j}(\ell)\mathbf{I}_{g_j(\ell)}$ for all $i \in \{1, \dots, \ell\}$ and $j \in \{1, \dots, m\}$. For all $j \in \{1, \dots, m\}$, we also have the spectral decomposition

$$oldsymbol{A}_{j}oldsymbol{W}_{\ell+1}oldsymbol{A}_{j}^{ op} = \sum_{h=1}^{u_{j}} b_{\ell+1,j,h}oldsymbol{A}_{j,h}^{ op}oldsymbol{A}_{j,h},$$

where $\mathbf{Q}_{j,h} = \mathbf{A}_{j,h}^{\top} \mathbf{A}_{j,h}$ for all $h \in \{1, ..., u_j\}$ and $j \in \{1, ..., m\}$, are orthogonal projection matrices that are mutually orthogonal, with ranks $g_{j,h}$, respectively. Since $\mathbf{Q}_{j,1} + \cdots + \mathbf{Q}_{j,u_j} = \mathbf{I}_{g_j}$, we have $g_{j,1} + \cdots + g_{j,u_j} = g_j$ for all $j \in \{1, ..., m\}$, as

well as $N = g_1 + \cdots + g_m$. We now take $\overline{A}_{j,h} = A_{j,h}A_j$ for all $h \in \{1, \ldots, u_j\}$ and $j \in \{1, \ldots, m\}$ so that, if $i \leq \ell$,

$$\overline{\boldsymbol{A}}_{j,h}\boldsymbol{W}_{i}\overline{\boldsymbol{A}}_{j,h}^{\top} = \boldsymbol{A}_{j,h}\boldsymbol{A}_{j}\boldsymbol{W}_{i}\boldsymbol{A}_{j}^{\top}\boldsymbol{A}_{j,h}^{\top} = \boldsymbol{A}_{j,h}(b_{i,j,h}\boldsymbol{I}_{g_{j}})\boldsymbol{A}_{j,h}^{\top} = b_{i,j,h}\boldsymbol{I}_{g_{j,h}},$$

for all $h \in \{1, ..., u_j\}$ and $j \in \{1, ..., m\}$. Moreover

$$\overline{\boldsymbol{A}}_{j,h}\boldsymbol{W}_{\ell+1}\overline{\boldsymbol{A}}_{j,h}^{\top} = \boldsymbol{A}_{j,h}(\boldsymbol{A}_{j}\boldsymbol{W}_{\ell+1}\boldsymbol{A}_{j}^{\top})\boldsymbol{A}_{j,h}^{\top} = \boldsymbol{A}_{j,h}\sum_{h'=1}^{n_{j}}(b_{\ell+1,j,h'}\boldsymbol{A}_{j,h'}^{\top}\boldsymbol{A}_{j,h'})\boldsymbol{A}_{j,h}^{\top} = b_{\ell+1,j,h}\boldsymbol{I}_{g_{j,h}}$$

since $\mathbf{A}_{j,h}\mathbf{A}_{j,h'}^{\top} = \mathbf{0}_{g_{j,h} \times g_{j,h'}}$, when $h \neq h'$.

To complete the proof we need only point out that $\mathbf{A}_j = [\overline{\mathbf{A}}_{j,1} \cdots \overline{\mathbf{A}}_{j,u_j}]^\top$ for all $j \in \{1, \ldots, m\}$. So we may take $\mathbf{P}_{\ell+1} = [\overline{\mathbf{A}}_{1,1}^\top \cdots \overline{\mathbf{A}}_{m,u_m}^\top]^\top$, which establishes the claim. \Box

The distinction between these results and those for families of commutative matrices is that in general

$$\forall_{j\neq j'} \quad \boldsymbol{A}_j \left(\sum_{i=1}^w c_i \boldsymbol{W}_i\right) \boldsymbol{A}_{j'}^\top \neq \boldsymbol{0}_{g_j \times g_{j'}}.$$

We say that the matrix $\boldsymbol{P} = [\boldsymbol{A}_1^\top \cdots \boldsymbol{A}_m^\top]^\top$, given by this proposition, is associated to the partition of the ADD model, with $\boldsymbol{V}(\boldsymbol{\theta}) = \sum_{i=1}^w \theta_i \boldsymbol{M}_i$, where $\boldsymbol{\theta} = [\theta_1 \cdots \theta_w]^\top$. In our approach we will use, for each $j \in \{1, \ldots, m\}$, the sub-model

$$Y_j = A_j Y \tag{2}$$

with mean vector $\boldsymbol{\mu}_j = \boldsymbol{X}_{0,j}\boldsymbol{\beta}_0$, where $\boldsymbol{X}_{0,j} = \boldsymbol{A}_j\boldsymbol{X}_0$, and variance–covariance matrix $\boldsymbol{V}(\boldsymbol{Y}_j) = \boldsymbol{\gamma}_j \boldsymbol{I}_{g_j}$, with $\boldsymbol{\gamma}_j = b_{1,j}\theta_i + \dots + b_{w,j}\theta_i$, where the $b_{i,j}$ are the coefficients in the statement of Proposition 1.

2.2. Estimation of variance components

For each $j \in \{1, ..., m\}$, let P_j and P_j^c be the orthogonal projection matrix on $\Omega_j = R(X_{0,j})$ and on its orthogonal complement Ω_j^{\perp} , respectively. Given

$$\forall_{j \in \{1,\dots,m\}} \quad p_j = \operatorname{rank}(\boldsymbol{P}_j), \quad p_j^c = \operatorname{rank}(\boldsymbol{P}_j^c) \tag{3}$$

we set $C = \{j : p_j > 0\}$ and $D = \{j : p_j^c > 0\}$. Since Y_1, \ldots, Y_m are homoscedastic, if $j \in D$ it is well known that, for each $j \in D$,

$$\widetilde{\boldsymbol{\gamma}}_{j} = \boldsymbol{Y}_{j}^{\top} \boldsymbol{P}_{j}^{c} \boldsymbol{Y}_{j} / p_{j}^{c} \tag{4}$$

is BQUE_(Y_j), i.e., it is the best quadratic unbiased estimators, in the family of the quadratic estimators of γ_j derived from Y_j . Let $\gamma(2)$ have components γ_j with $j \in \mathcal{D}$ and B(2) have as column vectors the column vectors of B with indexes in \mathcal{D} . Then $\gamma(2) = B(2)^{\top} \theta$. So if the row vectors of B(2) are linearly independent we get

$$\boldsymbol{\theta} = (\boldsymbol{B}(2)^{\top})^+ \boldsymbol{\gamma}(2),$$

where A^+ indicates the Moore–Penrose inverse of matrix A. We have $(B(2)^{\top})^+ = (B(2)B(2)^{\top})^+ B(2)$, so

$$\widetilde{\boldsymbol{\theta}} = (\boldsymbol{B}(2)^{\top})^{+} \widetilde{\boldsymbol{\gamma}}(2),$$

where the components of $\widetilde{\gamma}(2)$ are the $\widetilde{\gamma}(j)$ with $j \in \mathcal{D}$, is a least square estimator, LSE, since $\widetilde{\theta}$ minimizes

$$\mathbf{s}(\mathbf{v}) = \|\widetilde{\mathbf{y}}(2) - \mathbf{B}(2)^{\top}\mathbf{v}\|^2.$$

2.3. Estimable vectors

Let $\psi = G\beta_0$ be an estimable vector. Since we were able to estimate θ we can use the GLS estimator

$$\boldsymbol{\beta}_0(\widetilde{\boldsymbol{\theta}}) = (\boldsymbol{X}_0^\top \boldsymbol{V}(\widetilde{\boldsymbol{\theta}})^+ \boldsymbol{X}_0)^+ \boldsymbol{X}_0^\top \boldsymbol{V}(\widetilde{\boldsymbol{\theta}})^+ \boldsymbol{Y}_0$$

with

$$\boldsymbol{V}(\widetilde{\boldsymbol{\theta}}) = \sum_{i=1}^{w} \widetilde{\theta}_i \boldsymbol{M}_i,$$

to obtain $\widetilde{\psi}(\widetilde{\theta}) = G\beta_0(\widetilde{\theta})$.

(5)

3. Confidence regions and tests for variance components

If normality is assumed, we may use inducing pivot variables to obtain confidence intervals; see [10]. For each $j \in D$, let $\chi_{j,1}^2, \ldots, \chi_{j,N}^2$ be independent central chi-squares with g_j degrees of freedom. We then get the samples $\{\tilde{\theta}_{i,1}, \ldots, \tilde{\theta}_{i,N}\}$ for each $i \in \{1, \ldots, w\}$ with

$$\widetilde{\theta}_{i,N} = \sum_{j \in \mathcal{D}} a_{i,j} \frac{\mathbf{Y}^{\top} \mathbf{P}_{j}^{c} \mathbf{Y}}{\chi_{j,u}^{2}}$$

for each $u \in \{1, ..., N\}$ and $[a_{i,i}] = (\mathbf{B}(2)^{\top})^+$.

The empirical quantiles $\theta_{1,p,u}^*, \ldots, \theta_{w,p,u}^*$ of these samples strongly converge to the corresponding exact quantiles of the distribution induced for the variance components when $N \to \infty$; see again [10]. Then we get the induced 1 - q level confidence intervals $[\theta_{i,\frac{q}{2},N}^*; \theta_{i,1-\frac{q}{2},N}^*], [\theta_{i,q,N}^*; +\infty[, [0; \theta_{i,1-q,N}^*]]$ for all $i \in \{1, \ldots, w\}$ for the variance components, which enables us to test through duality the null hypothesis

$$\mathcal{H}_0: \forall_{i \in \{1, \dots, w\}} \ \theta_i = \theta_{0, i}.$$

4. Numerical example

In this section we present an example of a mixed model in which the relation matrices do not commute and illustrate the estimation of the variance components using ADD models. In addition, we compare the estimates of variance components obtained by our treatment with the ones obtained by the ANOVA method. As we will see, our treatment was more accurate in more than 80% of the time. Besides this, we obtain confidence intervals for the variance components and calculate their coverage probabilities.

We considered the linear model described in (1), with w = 3 and N = 8 simulated observations, viz.

$$\boldsymbol{Y} = \boldsymbol{X}_0\boldsymbol{\beta}_0 + \boldsymbol{X}_1\boldsymbol{\beta}_1 + \boldsymbol{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon},$$

with β_0 fixed and β_1 , β_2 and $\varepsilon = \beta_3$ independent and normally distributed, with null mean vectors and variance-covariance matrices $V(\beta_1) = \theta_1 I_2$, $V(\beta_2) = \theta_2 I_3$ and $V(\varepsilon) = \theta_3 I_8$. Thus Y has mean vector $\mu = X_0 \beta_0$, and variance-covariance matrix $V(Y) = \theta_1 M_1 + \theta_2 M_2 + \theta_3 M_3$, with $M_i = X_i X_i^{\top}$ for all $i \in \{1, 2, 3\}$. As design matrices we considered

$$\begin{split} \boldsymbol{X}_{0} &= \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}^{\top}, \\ \boldsymbol{X}_{1} &= \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}^{\top}, \quad \boldsymbol{X}_{2} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}^{\top} \end{split}$$

and $X_3 = I_8$.

In order to obtain the orthogonal matrix $P = [A_1^\top \cdots A_m^\top]^\top$, defined in Proposition 1, associated to the ADD model, we considered the orthogonal matrix $\dot{P} = [\dot{A}_1^\top \cdots \dot{A}_4^\top]^\top$, with

$$\dot{\mathbf{A}}_{1} = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} & 0 & 0 & 0 & 0 \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 1/\sqrt{6} & -2/\sqrt{6} & 1/\sqrt{6} & 0 & 0 & 0 & 0 \end{bmatrix}, \quad \dot{\mathbf{A}}_{2} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix},$$
$$\dot{\mathbf{A}}_{3} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \end{bmatrix}, \quad \dot{\mathbf{A}}_{4} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

Then, following Proposition 1, we did the spectral decomposition $\dot{A}_i M_1 \dot{A}_i^{\top}$ for $j \in \{1, \ldots, 4\}$ and obtained

$$\bar{\mathbf{A}}_{1,1} = \begin{bmatrix} 0.5773 & 0.5773 & 0.5773 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad \bar{\mathbf{A}}_{2,1} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0.5 & 0.5 & 0.5 \\ \bar{\mathbf{A}}_{2,2} = \begin{bmatrix} 0 & 0 & 0 & -0.5 & -0.5 & 0.5 & 0.5 \end{bmatrix}, \quad \bar{\mathbf{A}}_{3,1} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}, \\ \bar{\mathbf{A}}_{4,1} = \begin{bmatrix} 0.2581 & -0.5163 & 0.2581 & 0 & 0.3872 & -0.3872 & 0.3872 & -0.3872 \end{bmatrix}$$

and

$$\bar{A}_{4,2} = \begin{bmatrix} -0.7071 & 0 & 0.7.0710 & 0 & 0 & 0 & 0 \\ -0.3162 & 0.6324 & -0.3162 & 0 & 0.3162 & -0.3162 & 0.3162 & -0.3162 \\ 0 & 0 & 0 & 0.5 & -0.5 & -0.5 & 0.5 \end{bmatrix}$$

To simplify writing we considered the orthogonal matrix $\boldsymbol{P} = [\boldsymbol{A}_1^\top \cdots \boldsymbol{A}_6^\top]$, with $\boldsymbol{A}_1 = \bar{\boldsymbol{A}}_{1,1}, \boldsymbol{A}_2 = \bar{\boldsymbol{A}}_{2,1}, \boldsymbol{A}_3 = \bar{\boldsymbol{A}}_{2,2}, \boldsymbol{A}_4 = \bar{\boldsymbol{A}}_{3,1}$ $A_5 = A_{4,1}$ and $A_6 = A_{4,2}$.

At this point we used the software R to simulate several observation vectors as follows. We considered $\theta_3 = 1$ and θ_1 and θ_2 taking values in {0.25, 0.5, 1, 2, 4, 8, 16}. All possible combinations of θ_1 and θ_2 were considered. So, in whole,

Table 1
Averages of the variance components estimates obtained using the ADD method

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$;
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$,
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5.1967
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$).2350
$ ilde{ heta}_1$ 0.1505 0.3943 1.0789 2.0489 3.8426 8.2519 10).9763
$0.50 \tilde{\theta}_{2} \qquad 0.4800 0.5126 0.4502 0.5270 0.4871 0.5040 0$	5.1314
).4630
$\tilde{ heta}_3$ 1.0365 1.0630 0.9864 1.0029 0.9908 1.0227	1.0243
$ ilde{ heta}_1$ 0.2481 0.4807 0.9675 2.0491 3.9157 7.5792 1.4	1.2643
1 $ ilde{ heta}_2$ 0.9677 1.0165 0.9720 0.8909 1.0109 0.9829	1.0003
$ ilde{ heta}_3$ 0.9985 0.9908 0.9376 0.9984 0.9940 0.9514).9611
$ ilde{ heta}_1$ 0.2976 0.4861 1.0930 1.9224 4.1529 8.0903 14	5.7445
2 $\tilde{ heta}_2$ 1.9503 1.8220 1.8753 1.8624 2.0218 1.9666 $\tilde{ heta}$	2.0325
$ ilde{ heta}_3$ 0.9864 1.0043 0.9733 1.0028 0.9678 0.9786).9946
$ ilde{ heta}_1$ 0.2240 0.4160 0.9611 2.0463 3.9795 8.2095 12	5.8604
4 $\tilde{ heta}_2$ 4.2071 4.0616 3.8739 4.3060 3.9835 3.9604	4.0136
$\tilde{ heta}_3$ 1.0394 0.9794 1.0276 1.0415 1.0024 0.9709	1.0496
$ ilde{ heta}_1$ 0.2608 0.5117 0.8715 2.0893 3.8556 7.9237 16	5.9263
8 $ ilde{ heta}_2$ 8.1013 7.9765 7.9948 7.7734 7.9198 7.5978 8	3.0849
$ ilde{ heta}_3$ 1.0063 1.0170 1.0056 0.9957 0.9879 0.9972	1.0303
$ ilde{ heta}_1$ 0.2407 0.5481 1.0446 2.0339 4.1406 7.8557 1.	5.6787
16 $ ilde{ heta}_2$ 16.5753 16.5058 17.0812 15.0608 15.8374 15.5055 19	5.7250
$\tilde{ heta}_3$ 0.9842 1.0303 0.9842 1.0032 0.9710 1.0021).9705

we simulated 49 observation vectors. Then, for each observation vector, we randomly generated β_1 , β_2 and ε , with $\beta_1 \sim \mathcal{N}(\mathbf{0}, \theta_1 \mathbf{I}_2), \beta_2 \sim \mathcal{N}(\mathbf{0}, \theta_2 \mathbf{I}_3)$ and $\varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_8)$ and obtained the sub-models stated in (2), viz. $\mathbf{Y}_i = \mathbf{A}_i \mathbf{Y}$.

In addition, again for each observation vector, we obtained the orthogonal projection matrices P_j and P_j^c and the p_j and p_j^c for all $j \in \{1, ..., 6\}$, stated in (3). The results were $p_1^c = 0$, $p_2^c = 0$, $p_3^c = 1$, $p_4^c = 0$, $p_5^c = 1$ and $p_6^c = 3$. So in (4) we considered p_3^c , p_5^c and p_6^c .

Finally we obtained the estimates of the variance components using the estimator $\tilde{\theta}$ stated in (5). We proceeded this way 1000 times and obtained the averages for each case, $\theta_{ADD,i}$ for $i \in \{1, 2, 3\}$, which may be seen in Table 1.

As it may be seen, the obtained estimates are close to the previously considered θ_1 , θ_2 and θ_3 suggesting that ADD models may be taken into account for estimating variance components in models in which the relation matrices may not commute.

In order to obtain confidence intervals for the variance components, we generated central chi-squares $\chi_{i,u}^2$ for all $i \in \{1, 2, 3\}$ and $u \in \{1, ..., 1000\}$ with $g_1 = p_3^c$, $g_2 = p_5^c$ and $g_3 = p_6^c$ degrees of freedom, getting the samples $\{\tilde{\theta}_{i,1}, \ldots, \tilde{\theta}_{i,1000}\}$ for $i \in \{1, 2, 3\}$, with $\tilde{\theta}_{i,u}$. Finally, from these samples we got the 95% level confidence intervals, with lower and upper limits presented in Tables 2 and 3, respectively. So, for example for the previously considered $\theta_1 = 16$, $\theta_2 = 0.25$ and $\theta_3 = 1$, we have the estimates $\tilde{\theta}_1 = 16.1967$, $\tilde{\theta}_2 = 0.2350$ and $\tilde{\theta}_3 = 9763$ and the respective 95% level confidence intervals [12.4543, 21.9397], [0.1557, 0.3654] and [0.8372, 1.1548]. Table 4 shows the number of times, in percentages, the previously considered values were within the obtained confidence intervals. As it may be seen, the coverage probabilities are all close to 95%.

Table 5 shows the obtained averages of the variance components estimates using the ANOVA method, $\theta_{ANOVA,i}$ for $i \in \{1, 2, 3\}$. This estimates were obtained following [23]. To simplify the comparison with the estimates in Table 1 we calculated $\|\theta_i - \theta_{ANOVA,i}\|$ and $\|\theta_i - \theta_{ADD,i}\|$ for $i \in \{1, 2, 3\}$, for each case. The results for the difference $\|\theta_i - \theta_{ANOVA,i}\| - \|\theta_i - \theta_{ADD,i}\|$ for $i \in \{1, 2, 3\}$, for each case, are presented in Table 6. The negative values are presented in bold. As we can see, more than 80% of the values are positive which means that the ADD method produced more accurate estimates than the ANOVA method in more than 80% of the time (122 in 147 times). Besides this, we calculated the root-mean-square-error, RMSE, for the two methods, obtaining

RMSE_{ADD} =
$$\sqrt{\sum_{r=1}^{7} \sum_{s=1}^{7} \sum_{i=1}^{3} \frac{(\tilde{\theta}_{ADD,i,s,r} - \theta_{i,s,r})^2}{147}} = 0.34$$

and

RMSE_{ANOVA} =
$$\sqrt{\sum_{r=1}^{7} \sum_{s=1}^{7} \sum_{i=1}^{3} \frac{(\tilde{\theta}_{ANOVA,i,s,r} - \theta_{i,s,r})^2}{147}} = 0.80.$$

Table 2	
Lower limits of the 95% level confidence i	ntervals for the variance components

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	0.2217	0.2887	0.7667	1.5137	2.8345	6.3122	12.4543
0.25	$\tilde{\theta}_2$	0.1638	0.1769	0.1584	0.1782	0.2063	0.1746	0.1557
	$\tilde{\theta}_3$	0.8314	0.8546	0.8442	0.8458	0.8190	0.8070	0.8372
	$\tilde{\theta}_1$	0.0715	0.2579	0.7888	1.5381	2.9226	6.3167	12.3999
0.50	$\tilde{\theta}_2$	0.3429	0.3678	0.3220	0.3797	0.3500	0.3614	0.3309
	$\tilde{\theta}_3$	0.8883	0.9116	0.8453	0.8597	0.8489	0.8763	0.8783
	$\tilde{\theta}_1$	0.1491	0.3284	0.7052	1.5366	2.9762	5.8055	10.9707
1	$\tilde{\theta}_2$	0.7211	0.7581	0.7256	0.6614	0.7543	0.7340	0.7461
	$\tilde{\theta}_3$	0.8559	0.8489	0.8036	0.8551	0.8520	0.8155	0.8237
	$\tilde{\theta}_1$	0.1873	0.3316	0.8006	1.4390	3.1593	6.2023	12.8774
2	$\tilde{\theta}_2$	1.4787	1.3790	1.4213	1.4109	1.5335	1.4945	1.5419
2	$\tilde{\theta}_3$	0.8457	0.8607	0.8346	0.8592	0.8289	0.8389	0.8518
	$\tilde{\theta}_1$	0.1280	0.2793	0.6967	1.5333	3.0241	6.2921	12.1941
4	$\tilde{\theta}_2$	3.2158	3.1065	2.9632	3.2937	3.0459	3.0340	3.0696
	$\tilde{\theta}_3$	0.8907	0.8391	0.8806	0.8925	0.8591	0.8323	0.8996
	$\tilde{\theta}_1$	0.1580	0.3505	0.6286	1.5700	2.9320	6.0704	13.0205
8	$\tilde{\theta}_2$	6.2119	6.1245	6.1284	5.9710	6.0795	5.8357	6.2077
	$\tilde{\theta}_3$	0.8621	0.8714	0.8618	0.8535	0.8466	0.8543	0.8832
	$\tilde{\theta}_1$	0.1437	0.3783	0.7640	1.5256	3.1519	6.0202	12.0434
16	$\tilde{\theta}_2$	12.7644	12.6943	13.1490	11.5940	12.1797	11.9081	12.1013
	$\tilde{\theta}_3$	0.8436	0.8828	0.8433	0.8598	0.8323	0.8588	0.8315

 Table 3

 Upper limits of the 95% level confidence intervals for the variance components.

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	0.5418	0.6610	1.4981	2.8047	5.5343	11.1904	21.9397
0.25	$\tilde{\theta}_2$	0.3790	0.4040	0.3717	0.4044	0.3754	0.3955	0.3654
	$\tilde{ heta}_3$	1.1469	1.1790	1.1642	1.1672	1.1475	1.1131	1.1548
	$\tilde{\theta}_1$	0.2900	0.6210	1.5407	2.8488	5.4234	11.2166	21.8475
0.50	$\tilde{\theta}_2$	0.6990	0.7461	0.6572	0.7605	0.6553	0.7322	0.6753
	$\tilde{ heta}_3$	1.2253	1.2568	1.1660	1.1855	1.2132	1.2088	1.2109
	$\tilde{\theta}_1$	0.4183	0.7309	1.3826	2.8469	5.6413	10.3243	19.2892
1	$\tilde{\theta}_2$	1.3548	1.4206	1.3582	1.2542	1.4241	1.3749	1.3970
	$\tilde{\theta}_3$	1.1804	1.1710	1.1083	1.1803	1.1987	1.1253	1.1371
	$\tilde{\theta}_1$	0.4833	0.7377	1.5562	2.6761	5.5953	10.9946	22.6971
2	$\tilde{\theta}_2$	2.6840	2.5061	2.5769	2.5651	2.6519	2.7031	2.7883
2	$\tilde{\theta}_3$	1.1662	1.1879	1.1508	1.1849	1.1852	1.1565	1.1763
	$\tilde{\theta}_1$	0.3886	0.6432	1.3823	2.8490	5.2841	11.1483	21.4513
4	$\tilde{\theta}_2$	5.7178	5.5230	5.2773	5.8688	5.2884	5.3910	5.4636
	$\tilde{\theta}_3$	1.2287	1.1586	1.2150	1.2311	1.1791	1.1478	1.2412
	$\tilde{ heta}_1$	0.4346	0.7738	1.2590	2.9035	5.5772	10.7623	22.9245
8	$\tilde{\theta}_2$	10.9705	10.7992	10.8343	10.5388	10.9112	10.2996	10.9586
	$\tilde{ heta}_3$	1.1894	1.2020	1.1890	1.1775	1.1511	1.1793	1.2178
	$\tilde{\theta}_1$	0.4061	0.8262	1.4925	2.8269	5.6296	10.6861	21.2215
16	$\tilde{\theta}_2$	22.4124	22.3199	23.1048	20.3581	23.4361	20.9614	21.2756
	$\tilde{ heta}_3$	1.1636	1.2183	1.1637	1.1854	1.1687	1.1849	1.1479

Due to the data being obtained assuming normality, we also present, in Tables 7 and 8, the obtained averages of the variance components estimates, using the REML and ML method, respectively. As it may be seen, while the REML method gave quite good estimates except for 0.25, the ML method gave not so good ones, especially when $\theta_1 = 16$ or $\theta_2 = 16$.

Table 4

Number of times, in percentages, the previously considered value was within the obtained confidence interval.

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	92.8	94.0	93.7	96.3	96.9	97.2	96.5
0.25	$\tilde{\theta}_2$	93.9	93.3	93.1	92.0	92.1	95.0	93.1
	$\tilde{\theta}_3$	96.9	96.3	96.7	96.8	95.7	96.8	97.0
	$\tilde{\theta}_1$	93.2	93.7	94.7	94.9	97.3	97.0	96.8
0.50	$\tilde{\theta}_2$	94.1	93.8	94.2	96.1	94.2	93.7	94.7
	$\tilde{\theta}_3$	96.9	97.2	96.6	96.9	96.3	97.0	97.0
	$\tilde{\theta}_1$	91.0	94.6	95.5	96.2	97.2	96.4	96.9
1	$\tilde{\theta}_2$	94.3	95.3	95.6	95.9	96.0	94.6	94.7
	$\tilde{\theta}_3$	96.7	96.7	96.8	97.0	96.6	97.1	95.9
	$\tilde{\theta}_1$	92.9	93.6	94.0	94.9	95.7	97.1	97.5
2	$\tilde{\theta}_2$	95.5	96.3	95.0	95.4	96.0	95.9	96.7
	$\tilde{\theta}_3$	97.1	96.9	96.2	95.8	96.3	96.8	96.6
	$\tilde{\theta}_1$	93.2	94.3	94.0	94.8	95.0	97.1	97.4
4	$\tilde{\theta}_2$	95.7	96.6	96.1	96.9	96.2	96.4	96.1
	$\tilde{\theta}_3$	96.2	97.1	96.8	97.2	96.7	96.3	97.3
	$\tilde{\theta}_1$	93.7	94.3	95.2	95.4	95.5	95.8	96.7
8	$\tilde{\theta}_2$	96.0	95.8	95.7	95.9	95.7	96.2	97.6
	$\tilde{\theta}_3$	96.2	95.1	95.9	96.0	96.7	96.8	97.4
	$\tilde{\theta}_1$	92.7	93.1	94.8	96.6	96.3	97.0	97.6
16	$\tilde{\theta}_2$	96.5	96.0	95.9	95.6	96.4	96.9	96.6
	$\tilde{\theta}_3$	96.2	97.2	96.3	95.7	96.8	97.7	96.8

Table 5

Obtained averages of the variance components estimates using the ANOVA method.

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	0.2471	0.4872	0.9682	2.2342	4.3115	8.1144	15.1655
0.25	$\tilde{\theta}_2$	0.2719	0.2786	0.2666	0.3144	0.2370	0.2596	0.2730
	$\tilde{\theta}_3$	0.9826	0.9812	0.9604	0.9568	0.9495	1.0255	0.9560
	$\tilde{\theta}_1$	0.3517	0.5479	1.1170	2.0733	4.2713	6.3503	17.7927
0.50	$\tilde{\theta}_2$	0.5887	0.6017	0.6890	0.5759	0.5254	0.1110	0.7434
	$\tilde{\theta}_3$	0.8109	0.8439	0.8957	1.0267	0.8510	1.5620	0.8488
	$\tilde{\theta}_1$	0.2515	0.5391	1.0701	1.6647	4.1256	7.2296	19.3257
1	$\tilde{\theta}_2$	1.0948	1.0569	0.9143	0.9416	1.0094	0.7707	0.8007
	$\tilde{\theta}_3$	0.9264	0.9097	0.7965	1.1934	0.8746	1.2121	1.2071
	$\tilde{\theta}_1$	0.2355	0.5199	0.9740	2.1166	3.7247	8.4104	16.5201
2	$\tilde{\theta}_2$	2.1137	2.2072	1.9391	1.4614	2.2688	2.1558	2.3242
	$\tilde{\theta}_3$	0.9714	1.1932	1.0179	1.2992	0.7752	1.1844	0.5927
	$\tilde{\theta}_1$	0.1503	0.6923	0.8323	2.4440	3.6073	7.8223	17.6324
4	$\tilde{\theta}_2$	3.4113	4.2655	3.3875	4.2446	3.7503	3.3424	4.6038
	$\tilde{\theta}_3$	1.1041	0.8257	1.0476	0.8915	1.2818	1.0561	0.2838
	$\tilde{\theta}_1$	0.8507	0.8346	0.7432	2.0681	3.7691	9.9474	16.5953
8	$\tilde{\theta}_2$	8.3085	9.0133	8.5894	8.0086	8.7245	11.6922	8.5680
	$\tilde{\theta}_3$	0.5280	0.7308	1.6159	0.8827	0.7658	-0.1228	0.7241
	$\tilde{\theta}_1$	0.4042	0.8716	0.6665	2.2103	4.1267	8.3139	15.9530
16	$\tilde{\theta}_2$	19.5547	17.4413	17.3099	16.2097	19.6381	12.6995	15.8605
	$\tilde{\theta}_3$	0.7731	0.7554	1.2919	0.8285	0.4472	1.0528	1.8509

5. Final comments

Mixed models in which the relation matrices commute have interesting properties but imply requirements that are not met, for instance when there are missing observations. Thus it is interesting to study models where that may not happen. This is the case of ADD models.

Table 6 Results for the difference $\|\theta_i - \theta_{ANOVA,i}\| - \|\theta_i - \theta_{ADD,i}\|$ for $i \in \{1, 2, 3\}$.

				θ_1			
θ_2	0.25	0.50	1	2	4	8	16
$\tilde{\theta}_1$	-0.0888	-0.0580	-0.0166	0.2168	0.0423	-40.1221	0.6378
$\tilde{\theta}_2$	0.0168	0.0160	0.0054	0.0515	-0.0370	0.0017	0.0080
$ ilde{ heta}_3$	-0.0125	0.0160	0.0245	0.0306	0.0062	-0.0331	0.0204
$\tilde{\theta}_1$	0.0023	-0.0578	0.0380	0.0244	0.1139	1.3978	1.6613
$\tilde{ heta}_2$	0.0687	0.0891	0.1392	0.0489	0.0124	0.3850	0.2064
$ ilde{ heta}_3$	0.1526	0.0931	0.0907	0.0237	0.1398	0.5393	0.1269
$\tilde{\theta}_1$	-0.0004	0.0198	0.0376	0.2862	0.0413	0.3496	1.5900
$\tilde{\theta}_2$	0.0625	0.0404	0.0577	-0.0507	-0.0015	0.2121	0.1990
$\tilde{ heta}_3$	0.0721	0.0811	0.1411	0.1918	0.1194	0.1635	0.1682
$\tilde{\theta}_1$	-0.0331	0.0061	-0.0670	0.0390	0.1224	0.3200	-0.2244
$\tilde{\theta}_2$	0.0640	0.0292	-0.0638	0.4010	0.2470	0.1225	0.2916
$ ilde{ heta}_3$	0.0150	0.1889	-0.0088	0.2964	0.1926	0.1630	0.4019
$\tilde{\theta}_1$	0.0737	0.1084	0.1288	0.3977	0.3722	-0.0317	1.4928
$\tilde{\theta}_2$	0.3816	0.2039	0.4864	-0.0614	0.2332	0.6180	0.5902
$ ilde{ heta}_3$	0.0648	0.1537	0.0200	0.0669	0.2794	0.0270	0.6666
$ ilde{ heta}_1$	0.5899	0.3229	0.1283	-0.0212	0.0865	1.8711	-0.3310
$\tilde{\theta}_2$	0.2072	0.9898	0.5842	-0.2180	0.6444	3.2900	0.4830
$\tilde{ heta}_3$	0.4657	0.2522	0.6103	0.1130	0.2222	1.1200	0.2456
$\tilde{\theta}_1$	0.1449	0.3235	0.2889	0.1764	-0.0139	0.1696	-0.2743
$\tilde{\theta}_2$	2.9794	0.9355	0.2288	-0.7295	3.4755	2.8060	-0.1355
$\tilde{ heta}_3$	0.2111	0.2143	0.2761	0.1683	0.5238	0.0507	0.8215

Table 7

Obtained averages of the variance components estimates using REML method.

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	0.4615	0.6147	1.1511	2.0927	4.0977	8.0963	15.9047
0.25	$\tilde{\theta}_2$	0.3815	0.4126	0.3543	0.3529	0.3905	0.3482	0.3608
	$\tilde{ heta}_3$	0.7623	0.8097	0.8222	0.8663	0.9355	0.8338	0.8706
	$\tilde{\theta}_1$	0.4441	0.5696	1.2147	2.0838	4.2347	8.0603	17.1273
0.50	$\tilde{\theta}_2$	0.6478	0.5540	0.6181	0.6704	0.5331	0.5968	0.6410
	$\tilde{ heta}_3$	0.7632	0.8931	0.8093	0.8648	0.9407	0.9562	0.9069
	$\tilde{\theta}_1$	0.3884	0.6578	1.1744	2.2547	3.9207	7.9048	15.9257
1	$\tilde{\theta}_2$	0.9971	1.0199	1.2463	1.1512	1.1396	1.1340	1.2073
	$\tilde{\theta}_3$	0.8010	0.8451	0.8807	0.9124	0.8472	0.8424	0.9287
	$\tilde{\theta}_1$	0.4192	0.6788	1.1603	2.0397	3.6760	8.2923	16.3108
2	$\tilde{\theta}_2$	1.9677	1.9178	2.1376	2.0122	2.3089	1.9768	1.7288
	$\tilde{\theta}_3$	0.8231	0.8249	0.8930	0.9040	0.9730	0.9611	0.9425
	$\tilde{\theta}_1$	0.4077	0.6724	1.0714	2.0400	4.5518	8.5700	16.1926
4	$\tilde{\theta}_2$	3.9178	4.4286	3.9299	3.8472	3.9149	4.3336	4.1029
	$\tilde{\theta}_3$	0.8153	0.8564	0.8386	0.9538	0.9187	0.9821	0.9283
	$\tilde{\theta}_1$	0.4347	0.6652	0.9908	2.2400	3.8770	7.7192	16.0680
8	$\tilde{\theta}_2$	7.7689	7.8151	8.6458	7.9055	7.7903	8.0347	9.4192
	$\tilde{\theta}_3$	0.8103	0.8560	0.9335	0.9344	0.9720	0.9791	0.9956
	$\tilde{\theta}_1$	0.4244	0.6114	1.0301	1.8961	4.2420	8.4242	15.4403
16	$\tilde{\theta}_2$	16.4998	16.9996	15.0907	16.7635	16.0125	16.1999	15.9348
	$\tilde{ heta}_3$	0.8357	0.8648	0.9354	0.9708	0.9644	1.0229	0.9845

In this paper we presented a treatment for the estimation of variance components and estimable vectors in linear mixed models in which the relation matrices may not commute. Besides this we also obtained confidence regions and derived tests for hypothesis on variance components. We illustrated the theory with a numerical example, where the obtained results were quite good. We compared the estimates of variance components obtained with our treatment with the ones obtained using the ANOVA method in an unbalanced mixed model and our treatment produced more accurate results in more than 80% of the time. The REML and ML estimates were also obtained. As we have seen, the performance of our method was quite

Table 8

Obtained averages of the variance components estimates using ML method.

					θ_1			
θ_2		0.25	0.50	1	2	4	8	16
	$\tilde{\theta}_1$	0.2808	0.4364	0.8519	1.5558	3.0986	6.1459	12.8539
0.25	$\tilde{\theta}_2$	0.2931	0.2460	0.2047	0.2195	0.2041	0.2501	0.2734
	$\tilde{\theta}_3$	0.7728	0.8928	0.8349	0.9287	0.9978	1.0107	0.9277
	$\tilde{\theta}_1$	0.2515	0.5351	0.8919	1.6472	3.5298	6.2326	12.5241
0.50	$\tilde{\theta}_2$	0.4572	0.4847	0.6243	0.5985	0.3859	0.3992	0.4267
	$\tilde{\theta}_3$	0.8880	0.9210	0.8999	0.9619	0.9158	0.9420	0.9471
	$\tilde{\theta}_1$	0.2982	0.5005	0.8702	1.5418	3.0969	6.3442	12.8077
1	$\tilde{\theta}_2$	0.9450	0.9358	1.0730	1.0409	0.7933	1.2113	1.0980
	$\tilde{\theta}_3$	0.8221	0.9072	0.9168	0.9394	1.0339	0.9993	0.9890
	$\tilde{\theta}_1$	0.3007	0.5066	0.8660	1.7114	3.6039	6.7655	12.6275
2	$\tilde{\theta}_2$	1.9238	2.1981	1.9759	1.9803	2.1818	2.5245	1.4850
2	$\tilde{\theta}_3$	0.8178	0.9233	1.0522	1.0100	0.9999	1.0100	0.9810
	$\tilde{\theta}_1$	0.2642	0.4849	0.9107	1.8073	3.1637	6.9428	13.8888
4	$\tilde{\theta}_2$	3.8506	3.9155	4.3264	4.0651	4.1555	4.4530	3.0252
	$\tilde{\theta}_3$	0.8482	0.9168	0.9809	0.9888	0.9871	1.0141	0.9904
	$\tilde{\theta}_1$	0.3335	0.5179	0.9050	1.7350	3.5722	7.3558	13.4083
8	$\tilde{\theta}_2$	8.2176	8.4727	7.5814	8.5236	8.3920	8.7828	9.0678
	$\tilde{\theta}_3$	0.8401	0.8787	0.9558	1.0075	1.0045	1.0209	1.0311
	$\tilde{\theta}_1$	0.3386	0.4801	0.9276	1.8596	3.2791	7.2631	13.5366
16	$\tilde{\theta}_2$	13.2895	13.1011	13.2192	13.7911	13.8238	13.6894	13.0934
	$\tilde{\theta}_3$	0.8773	0.9453	0.9932	1.0442	0.9697	1.0225	1.0348

good and it has the advantage over the ML and REML methods of not requiring normality. Moreover, our method is a unified method contrary to the ANOVA methods.

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