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ON SOME PROPERTIES OF ML AND REML ESTIMATORS IN MIXED NORMAL MODELS WITH TWO VARIANCE COMPONENTS

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Abstract

In the paper, the problem of estimation of variance components σ_1^2 and σ_2^2 by using the ML-method and REML-method in a normal mixed linear model $\mathcal{N}\left\{Y, \mathrm{E}(Y) = X\beta, \,\mathrm{Cov}(Y) = \sigma_1^2 V + \sigma_2^2 I_n\right\}$ is considered. This paper deal with properties of estimators of variance components, particularly when an explicit form of these estimators is unknown. The conditions when the ML and REML estimators can be expressed in explicit forms are given, too. The simulation study for one-way classification unbalanced random model together with a new proposition of approximation of expectation and variances of ML and REML estimators are shown. Numerical calculations with reference to the generalized Fisher's information are also given.

Keywords: mixed linear models, likelihood-based inference, ML- and REML- estimation, variance components, Fisher's information.

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1. Introduction

Let us consider a normal mixed linear model $\mathcal{N}\{Y, X\beta, \Sigma(\sigma)\}$, in which Y is a normally distributed random R^n-vector with

$$\mathrm{E}(Y) = X\beta, \quad \mathrm{Cov}(Y) = \Sigma(\sigma) = \sigma_1^2 V + \sigma_2^2 I_n.$$

Here X is a known $n \times p$ matrix of rank p $(p < n)$, β is an unknown R^p-vector of fixed parameters, V is a known nonnegative definite matrix, I_n is the $n \times n$ identity matrix, while $\sigma = (\sigma_1^2, \sigma_2^2)'$ is a vector of unknown variance components belonging to $\mathcal{S} = \{\sigma : \sigma_1^2 \geq 0, \sigma_2^2 > 0\}$.

One of a possible method of estimation of σ in the above described model follows from the maximum likelihood (ML) principle. It is made using the profile log likelihood (for the observed y)

$$l = -\frac{1}{2} y' P_\Sigma y - \frac{1}{2} \log|\Sigma|,$$

where

$$P_\Sigma = \Sigma^{-1} - \Sigma^{-1} X (X'\Sigma^{-1} X)^{-1} X' \Sigma^{-1} = (M \Sigma M)^+,$$

$M = I_n - P$, $P = X(X'X)^{-1}X'$, while the symbol "+" denotes the Moore-Penrose inverse (see, e.g., Rao and Kleffe [11] p. 230). It is well known that ML estimators, when they exist, are generally heavily biased. For the one- and two-way classification models this problem has been considered in detail by Swallow and Monahan [17] and by Gnot *et al.* [5]. An adjusted version of the profile log likelihood l can be constructed by adding to l the term $-\frac{1}{2}\log|X'\Sigma^{-1}X|$. The estimators that maximize such an adjusted profile log likelihood

$$l_0 = -\frac{1}{2} y' P_\Sigma y - \frac{1}{2} \log|\Sigma| - \frac{1}{2} \log|X'\Sigma^{-1} X|$$

are known as the restricted or residual maximum likelihood (REML) estimators. The REMLEs obtained for the data vector y reduced to the least-squares residual vector $(I_n - P)y$ have been introduced by Patterson and Thompson [8], [9], (see also Caliński and Kageyama [2], Stern and Welsh [16] for more recent references). The question of the existence of maximum likelihood estimates for the parameter vector (β, σ), under more general types of constraints on the variance components than the usual nonnegativity, has been investigated by Birkes and Wulff [1].

2. A spectral form of the profile log likelihood functions - ML and REML equation systems

Another way which leads us to REML estimators is based on a model reduced by the invariance principle. Let B be an $(n-p) \times n$ matrix such that $BB' = I_{n-p}$ and $B'B = M$, $p = \text{rank}(X)$. Denote by $m_1 > ... > m_{d-1} > m_d = 0$ the ordered sequence of the different eigenvalues of BVB'. Let

$$BVB' = \sum_{i=1}^{d-1} m_i E_i$$

be the spectral decomposition of BVB', and let E_d be such that $\sum_{i=1}^{d} E_i = I_{n-p}$. Here the E_i's are orthogonal projectors such that $E_i E_j = 0$ for $i \neq j$. Consider the random vector $T = (T_1, T_2, ..., T_d)'$ with $T_i = z' E_i z / \nu_i, \quad z = By, \quad i = 1, ..., d$, where $\nu_1, ..., \nu_d$ are the multiplicities of m_i's. Note that the multiplicity ν_d of $m_d = 0$ is $\nu_d = n - p - \text{rank}(BVB')$. Observe that $\text{rank}(BVB') = \text{rank}(MVM)$. Throughout the paper we assume that $\nu_d > 0$.

Remark 2.1. Following Olsen *et al.* [7]), under normality of y, the random variables T_i's form a set of minimal sufficient and independent statistics for the reduced model $\mathcal{N}\{z, 0, \sigma_1^2 BVB' + \sigma_2^2 I_{n-p}\}$, and $\nu_i T_i / (m_i \sigma_1^2 + \sigma_2^2)$ for $i = 1, ..., d$ have the central chi-square distribution with ν_i degrees of freedom. The expectation and the variance of T_i are

$$\text{E}(T_i) = m_i \sigma_1^2 + \sigma_2^2,$$

$$\text{Var}(T_i) = \frac{2}{\nu_i} \left(m_i \sigma_1^2 + \sigma_2^2 \right)^2,$$

respectively.

Remark 2.2 (see, e.g., Ellbassiouni [3], Rao and Kleffe [11]). The REML estimator for σ in the original model $\mathcal{N}\{Y, X\beta, \Sigma(\sigma)) = \sigma_1^2 V + \sigma_2^2 I_n\}$ is the ML estimator for σ in the reduced model $\mathcal{N}\{z, 0, \Sigma_0(\sigma) = \sigma_1^2 BVB' + \sigma_2^2 I_{n-p}\}$.

Let $\alpha_1 > \alpha_2 >, ..., > \alpha_{d_0 - 1} > \alpha_{d_0} = 0$ be the eigenvalues of V with the multiplicities $s_1, s_2, ..., s_{d_0}$, respectively ($s_{d_0} = n - \text{rank}(V)$). It has been shown by Gnot *et al.* [5] that the log likelihood functions l and l_0 can be presented in a spectral form given in the following propositions.

Proposition 2.1. *The* log *likelihood functions*

$$l=-\frac{1}{2}y'(M\Sigma M)^{+}y-\frac{1}{2}\log|\Sigma|$$

and

$$l_0=-\frac{1}{2}y'\left(M\Sigma M\right)^{+}y-\frac{1}{2}\log|\Sigma_0|=-\frac{1}{2}t'B'\Sigma_0^{-1}Bt-\frac{1}{2}\log|\Sigma_0|$$

can be presented in the following spectral form

$$l=-\sum_{j=1}^{d_0}s_j\log\left(\alpha_j\sigma_1^2+\sigma_2^2\right)-\sum_{i=1}^{d}\frac{\nu_i}{m_i\sigma_1^2+\sigma_2^2}T_i. \tag{1}$$

$$l_0=-\sum_{j=1}^{d}\nu_j\log\left(m_j\sigma_1^2+\sigma_2^2\right)-\sum_{i=1}^{d}\frac{\nu_i}{m_i\sigma_1^2+\sigma_2^2}T_i. \tag{2}$$

Straightforward calculations lead to the following nonlinear (in general) ML and REML equation system.

Proposition 2.2. *ML and REML equation systems can be presented in the following spectral form, respectively*

$$\sum_{i=1}^{d-1}\frac{\nu_i m_i}{(m_i\sigma_1^2+\sigma_2^2)^2}T_i=\sum_{j=1}^{d_0-1}\frac{s_j\alpha_j}{\alpha_j\sigma_1^2+\sigma_2^2}, \tag{3}$$

$$\sum_{i=1}^{d}\frac{\nu_i}{(m_i\sigma_1^2+\sigma_2^2)^2}T_i=\sum_{j=1}^{d_0}\frac{s_j}{\alpha_j\sigma_1^2+\sigma_2^2}. \tag{4}$$

$$\sum_{i=1}^{d-1}\frac{\nu_i m_i}{(m_i\sigma_1^2+\sigma_2^2)^2}T_i=\sum_{j=1}^{d-1}\frac{\nu_j m_j}{m_j\sigma_1^2+\sigma_2^2}, \tag{5}$$

$$\sum_{i=1}^{d}\frac{\nu_i}{(m_i\sigma_1^2+\sigma_2^2)^2}T_i=\sum_{j=1}^{d}\frac{\nu_j}{m_j\sigma_1^2+\sigma_2^2}. \tag{6}$$

Notice that in the above equations the left hand sides of (3) and (4) are the same as the left hand sides of (5) and (6). Moreover, the right hand sides of expressions (5) and (6) are the expectations of the left hand side ones. This note gives us hope that biases of REML estimators should not be essential. A next important remark is that (3) and (4) is linear with respect to the variance components iff $d = d_0 = 2$ and $m_1 = \alpha_1$, while the system (5) and (6) becomes linear iff $d = 2$ (cf. Szatrowski [18], Szatrowski and Miller [19], Gnot *et al.* [4], [5]). If the above conditions hold, then ML and REML estimators can be expressed in explicit forms given by the following theorems.

Theorem 2.1. *If $d = d_0 = 2$ and $m_1 = \alpha_1$, then the ML estimator for σ_1^2 and σ_2^2 reduces to*

$$\hat{\sigma}^2_{1ML} = \frac{\nu_1}{m_1 s_1} T_1 - \frac{n - p - \nu_1}{m_1(n - s_1)} T_2, \tag{7}$$

$$\hat{\sigma}^2_{2ML} = \frac{n - p - \nu_1}{n - s_1} T_2. \tag{8}$$

The expectations and the variances of the estimators have the form

$$\mathrm{E}(\hat{\sigma}^2_{1ML}) = \frac{\nu_1}{s_1}\sigma_1^2 + \left(\frac{\nu_1}{m_1 s_1} - \frac{n - p - \nu_1}{m_1(n - s_1)}\right)\sigma_2^2, \tag{9}$$

$$\mathrm{E}(\hat{\sigma}^2_{2ML}) = \frac{n - p - \nu_1}{n - s_1}\sigma_2^2, \tag{10}$$

$$\mathrm{Var}(\hat{\sigma}^2_{1ML}) = \frac{1}{m_1^2}\left[\frac{2\nu_1}{s_1^2}(m_1\sigma_1^2 + \sigma_2^2)^2 + \frac{2(n - p - \nu_1)}{(n - s_1)^2}\sigma_2^4\right], \tag{11}$$

$$\mathrm{Var}(\hat{\sigma}^2_{2ML}) = \frac{2(n - p - \nu_1)}{(n - s_1)^2}\sigma_2^4. \tag{12}$$

Theorem 2.2. *If $d = 2$, then REML-estimators for σ_1^2 and σ_2^2 reduce uniformly to minimum variance unbiased ANOVA estimators being of the form*

$$\hat{\sigma}^2_{1REML} = \frac{1}{m_1}(T_1 - T_2), \tag{13}$$

$$\hat{\sigma}^2_{2REML} = T_2. \tag{14}$$

The REML estimators are unbiased and their variances have the form

$$\mathrm{Var}(\hat{\sigma}^2_{1REML}) = \frac{1}{m_1^2}\left[\frac{2}{\nu_1}(m_1\sigma_1^2 + \sigma_2^2)^2 + \frac{2\sigma_2^4}{n - p - \nu_1}\right], \tag{15}$$

$$\mathrm{Var}(\hat{\sigma}^2_{2REML}) = \frac{2\sigma_2^4}{n - p - \nu_1}. \tag{16}$$

3. Approximations of expectations and variances with Fisher's informations of ML and REML estimators

3.1. General remark

The conditions for the existence of ML or REML estimators in explicit forms are very restricted. For example, for a one-way classification random model

$$Y = \mathbf{1}_n\beta + \mathrm{diag}\{\mathbf{1}_{n_1}, ..., \mathbf{1}_{n_r}\}\gamma + \varepsilon, \tag{17}$$

(where $\gamma = (\gamma_1, ...\gamma_r)$ is a vector of random treatment effects and $\varepsilon = (\varepsilon_1, ..., \varepsilon_n)$ is a vector of uncorrelated random errors) with the following probabilistic structure on linear statistical normal space

$$\mathcal{N}\{Y, \mathrm{E}(Y) = \mathbf{1}_n\beta, \Sigma(\sigma) = \mathrm{diag}\{\mathbf{1}_{n_1}\mathbf{1}'_{n_1}, ..., \mathbf{1}_{n_r}\mathbf{1}'_{n_r}\}\sigma_1^2 + I_n\sigma_2^2\} \tag{18}$$

the conditions of Theorem 2.1 are satisfied iff the replications n_i in each $i-$th class, for $i = 1, ..., r$ are the same. However, the number of different eigenvalues of BVB' is $d = 2$ iff we have at most two unequal-replicated classes.

More details concerning this problem can be found in Elbassiouni [3] and in Gnot *et al.* [4], [5]. For the models in which the above conditions are not satisfied we have forced to use some iterative procedures proposed to solve ML and REML equations systems. There is rich literature in which several algorithms have been suggested to find a good numerical solution for the REML estimate, if it exists. Most of them such as the Newton-Raphson algotithm, Fisher's scoring method (REML estimator as an iterative version of MINQUE, see, e.g., Rao [10], Section 6.6 and 6.7), EM algorithm, and some contributions made by various authors (cf. Searle *et al.* [13], Section 8). Extraordinary useful are these procedures which allow us to control biases and variances of the estimators by simulation study.

Now, we would like to show how to get quite good approximations of these parameters without any simulations. Moreover, we show also the relationships between the approximations of variances for ML and REML estimators and the generalized information inequality.

3.2. Approximations for ML estimators

The approximations of the expectations and the variances of ML estimators can be taken from the formulas (9) to (12) by making suitable replacements, and so: m_1 by c, ν_1 by ν, s_1 by s, where $m \le c \le \alpha$,

$$\alpha = \frac{\sum_{i=1}^{d_0} s_i \alpha_i}{\sum_{i=1}^{d_0-1} s_i} = \frac{\mathrm{tr}(V)}{\mathrm{rank}(V)}, \quad s = \sum_{i=1}^{d_0-1} s_i = \mathrm{rank}(V),$$

$$m = \frac{\sum_{i=1}^{d} \nu_i m_i}{\sum_{i=1}^{d-1} \nu_i} = \frac{\mathrm{tr}(MVM)}{\mathrm{rank}(MVM)}, \quad \nu = \sum_{i=1}^{d-1} \nu_i = \mathrm{rank}(MVM).$$

If $d = d_0 = 2$ and $\alpha_1 = m_1$, then the approximated variances coincide with the expectations and the variances given by Theorem 2.1.

3.3. Approximations for REML estimators

Since the right hand sides of expressions (5) and (6) are the expectations of the left hand side ones, it should be expected that the biases of REML estimators of σ_1^2 and σ_2^2 are negligible. The approximations of variances of

REML estimators of σ can be taken from the formulas (15) and (16) by putting m and ν instead of m_1 and ν_1, respectively.

If $d = 2$, the approximated variances coincide with the variances of ANOVA estimators given by (15) and (16).

3.4. Fisher's information for ML and REML estimators

Let the terms $A(\sigma), B(\sigma), C(\sigma)$ and $A_0(\sigma), B_0(\sigma), C_0(\sigma)$ be the elements of information matrices for ML and REML estimators of $\sigma = (\sigma_1^2, \sigma_2^2)$ with the determinants given by $D(\sigma) = A(\sigma) \cdot B(\sigma) - C(\sigma)^2$ and $D_0(\sigma) = A_0(\sigma) \cdot B_0(\sigma) - C_0(\sigma)^2$, respectively. Then by straightforward calculations we have:

$$A(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l(\sigma)}{(\partial \sigma_1^2)^2} \right] = 2 \sum_{i=1}^{d-1} \frac{\nu_i m_i^2}{(m_i \sigma_1^2 + \sigma_2^2)^2} - \sum_{j=1}^{d_0-1} \frac{s_j \alpha_j^2}{(\alpha_j \sigma_1^2 + \sigma_2^2)^2},$$

$$B(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l(\sigma)}{(\partial \sigma_2^2)^2} \right] = 2 \sum_{i=1}^{d} \frac{\nu_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} - \sum_{j=1}^{d_0} \frac{s_j}{(\alpha_j \sigma_1^2 + \sigma_2^2)^2},$$

$$C(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l(\sigma)}{\partial \sigma_1^2 \partial \sigma_2^2} \right] = 2 \sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} - \sum_{j=1}^{d_0-1} \frac{s_j \alpha_j}{(\alpha_j \sigma_1^2 + \sigma_2^2)^2},$$

$$A_0(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l_0(\sigma)}{(\partial \sigma_1^2)^2} \right] = \sum_{i=1}^{d-1} \frac{\nu_i m_i^2}{(m_i \sigma_1^2 + \sigma_2^2)^2},$$

$$B_0(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l_0(\sigma)}{(\partial \sigma_2^2)^2} \right] = \sum_{i=1}^{d} \frac{\nu_i}{(m_i \sigma_1^2 + \sigma_2^2)^2},$$

$$C_0(\sigma) = \mathrm{E}_\sigma \left[-\frac{\partial^2 l_0(\sigma)}{\partial \sigma_1^2 \partial \sigma_2^2} \right] = \sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i \sigma_1^2 + \sigma_2^2)^2}.$$

Now, according to the generalized Cramér-Rao's inequality (see Lehman [6], Section 2) we obtain the following down bound for the variances of ML and REML estimators σ_1^2 and σ_2^2 without theirs biases, respectively:

$$\mathrm{Var}_{\inf}(\sigma^2_{1ML}) = \frac{B(\sigma)}{D(\sigma)}, \quad \mathrm{Var}_{\inf}(\sigma^2_{2ML}) = \frac{A(\sigma)}{D(\sigma)},$$

and

$$\mathrm{Var}_{\inf}(\sigma^2_{1REML}) = \frac{B_0(\sigma)}{D_0(\sigma)}, \quad \mathrm{Var}_{\inf}(\sigma^2_{2REML}) = \frac{A_0(\sigma)}{D_0(\sigma)}.$$

Note 3.1. Because we do not know exact biases $b(\sigma)$ of estimators σ therefore in our calculations of down bounds for variances the terms $[\frac{\partial b(\sigma)}{\partial \sigma_i^2}]^2$ for $i = 1, 2$ have been neglected.

4. Results of simulations and approximations

In this section, we use the results of simulations given by Swallow and Monahan [17] and our outcomes to compare approximations of the biases and the variances of REML and ML estimators of σ with those obtained from simulations in unbalanced one-way classification random models given by (17) and (18). For the model we will also use the same notation k-pattern numbers $P_k = (n_1, ..., n_r)$ for $k = 2, 12, 13$, with given replications n_i for $i-$th class and with total number of observations $n = \sum_{i=1}^{r} n_i$. For details concerning these models see e.g., Searle *et al.* [13], Section 3. The results of simulations and approximations for k-pattern numbers $P_2 = (1, 5, 9), P_{12} = (2, 10, 18)$ and $P_{13} = (3, 15, 27)$ are presented bellow in Tables 4.1, 4.4, 4.7 (ML estimation) and Tables 4.2, 4.5, 4.8 (REML estimation), respectively. In Tables 4.3, 4.6, 4.9 we present additionally the estimated probabilities for the positively determinate covariance matrix $\Sigma(\sigma)$ (ML estimation), $\Sigma_0(\sigma)$ (REML estimation) and the probabilities for values σ_1^2 from the natural parametric space $[0; \infty)$ in the studied k-pattern P_2, P_{12}, P_{13}, respectively. The selection of the above models allow us to obtain for REML estimators exact solutions of stochastic equation systems given by (5) and (6) as roots of a polynomial of third and fourth degree. On the other hand, we may study the influence of increasing replications on k-patterns: $P_{12} = 2 \cdot P_2, P_{13} = 3 \cdot P_2$.

Note 4.1. It is worth stressing that Σ and Σ_0 are positive definite, not only for $\sigma_1^2 \in [0, \infty)$, but for all $\theta = \sigma_1^2/\sigma_2^2 \in [-1/\alpha_1, \infty)$, where α_1 is the largest characteristic value of V (ML-estimation) and for $\theta \in [-1/m_1, \infty)$, where m_1 is the largest characteristic value of BVB' (REML-estimation). Since $\alpha_1 > m_1$, hence we have $P(\Sigma > 0) \leq P(\Sigma_0 > 0)$. Thus a model for y or By with $\Sigma = \sigma_2^2(\theta V + I_n)$ or with $\Sigma_0 = \sigma_2^2(\theta BVB' + I_n)$, respectively, is somewhat more flexible than the original model with $\sigma \in \bar{\mathcal{R}}_+ \times \mathcal{R}_+$. As discussed by, for example, Snedecor and Cochran ([15], Section 13.5) the models are better suited for certain applications than models with original parametric space for σ.

For a fixed $\sigma_1^2 = .0, .1, .2, .5, 1.0, 2.0, 5.0$ and $\sigma_2^2 = 1$ the tables 4.1–4.9 contain the following statistics:

- $\hat{\sigma}^2_{1(SM)}$ - sample means taken from simulations (Swallow and Monahan [17]),
- $\hat{\sigma}^2_1$ - sample means taken from our simulations,
- E^m_{ap} - approximated expectations of $\hat{\sigma}^2_1$ with $c = m$,
- E^α_{ap} - approximated expectations of $\hat{\sigma}^2_1$ with $c = \alpha$,
- Var_{SM} - sample variances of $\hat{\sigma}^2_1$ taken from simulations (Swallow and Monahan [17]),
- Var_{GMU} - sample variances of $\hat{\sigma}^2_1$ taken from our simulations,
- Var^m_{ap} - approximated variances of $\hat{\sigma}^2_1$ with $c = m$,
- Var^α_{ap} - approximated variances of $\hat{\sigma}^2_1$ with $c = \alpha$,
- $\mathrm{Var}_{\inf}(\sigma^2_1)$ - inverse of Fisher's information for component variance σ^2_1,
- $\hat{P}(\Sigma > 0)$ - estimated probabilities from simulations in the ML-method for regions of positive determinability of covariance matrix Σ,
- $\hat{P}(\sigma^2_1 > 0)$ - estimated probabilities from simulations for positive values of variance component σ^2_1,
- $\hat{P}(\Sigma_0 > 0)$ - estimated probabilities from simulations in the REML-method for regions of positive determinability of covariance matrix Σ_0.

Example 1. Characteristics of design for k-pattern P_2=(1, 5, 9).

n	p	α_1	α_2	α_3	s_4	m_1	m_2	m	α	ν_3	s	ν
15	1	9	5	1	12	6.477	1.389	3.933	5	12	3	2

n - number of observations;
p - rank(X);
α_i - eigenvalues of matrix V;
s_4 - multiplicity of zero eigenvalue of V;
m_i - eigenvalues of BVB';
ν_3 - multiplicity of zero eigenvalue of BVB';
m, α, s, ν are determined by formulas as in Subsection 3.2.

Table 4.1. The results of simulations and approximations of ML estimators of σ_1^2 for the model $P_2 = (1, 5, 9)$.

σ_1^2	$\hat{\sigma}_{1(SM)}^2$	$\hat{\sigma}_1^2$	E_{ap}^m	E_{ap}^α
.0	.036	.028	−.085	−.067
.1	.079	.085	−.018	.000
.2	.127	.133	.049	.067
.5	.298	.317	.249	.267
1.0	.611	.666	.582	.600
2.0	1.229	1.273	1.249	1.267
5.0	3.210	3.315	3.249	3.267

σ_1^2	Var_{SM}	Var_{GMU}	Var_{ap}^m	Var_{ap}^α	$\mathrm{Var}_{\inf}(\sigma_1^2)$
.0	.024	.025	.040	.024	.011
.1	.047	.043	.067	.047	.031
.2	.081	.080	.103	.078	.060
.5	.285	.279	.264	.224	.198
1.0	.834	.836	.710	.647	.576
2.0	2.442	2.445	2.269	2.158	1.854
5.0	12.966	12.981	12.281	12.024	9.717

Table 4.2. The results of simulations and approximations of REML estimators of σ_1^2 for the model $P_2 = (1, 5, 9)$.

σ_1^2	$\hat{\sigma}^2_{1(SM)}$	$\hat{\sigma}_1^2$	Var_{SM}	Var_{GMU}	Var^m_{ap}	Var^α_{ap}	$\mathrm{Var}_{inf}(\sigma_1^2)$
.0	.112	.045	.098	.110	.075	.047	.025
.1	.198	.138	.168	.189	.136	.098	.062
.2	.283	.244	.254	.299	.217	.168	.114
.5	.578	.539	.753	.785	.580	.498	.339
1.0	1.077	1.031	2.059	2.058	1.584	1.448	.928
2.0	2.036	2.030	5.672	5.851	5.092	2.848	2.864
5.0	5.035	5.033	28.810	29.300	27.618	27.048	14.676

Table 4.3. The estimated probabilities from simulations for regions of positive determinability of variance-covariance matrices Σ and Σ_0 and variance component σ_1^2 for the model $P_2 = (1, 5, 9)$.

σ_1^2	$ML - estimation$		$REML - estimation$	
	$\hat{P}(\Sigma > 0)$	$\hat{P}(\sigma_1^2 > 0)$	$\hat{P}(\Sigma_0 > 0)$	$\hat{P}(\sigma_1^2 > 0)$
.0	.620	.358	.623	.362
.1	.695	.479	.706	.480
.2	.747	.554	.749	.557
.5	.802	.671	.816	.678
1.0	.851	.760	.869	.770
2.0	.899	.842	.914	.846
5.0	.950	.919	.957	.923

Example 2. Characteristics of design for k-pattern P_{12}=(2, 10, 18).

n	p	α_1	α_2	α_3	s_4	m_1	m_2	m	α	ν_3	s	ν
30	1	18	10	2	27	12.954	2.779	7.867	10	27	3	2

n - number of observations;
p - rank(X);
α_i - eigenvalues of matrix V;
s_4 - multiplicity of zero eigenvalue of V;
m_i - eigenvalues of BVB';
ν_3 - multiplicity of zero eigenvalue of BVB';

m, α, s, ν are determined by formulas as in Subsection 3.2.

Table 4.4. The results of simulations and approximations of ML estimators of σ_1^2 for the model $P_{12} = (2, 10, 18)$.

σ_1^2	$\hat{\sigma}^2_{1(SM)}$	$\hat{\sigma}_1^2$	E^m_{ap}	E^α_{ap}
.0	.016	.015	−.042	−.033
.1	.062	.064	.024	.033
.2	.119	.121	.091	.100
.5	.300	.315	.291	.300
1.0	.628	.627	.624	.633
2.0	1.292	1.333	1.291	1.300
5.0	3.240	3.298	3.291	3.300

σ_1^2	Var_{SM}	Var_{GMU}	Var^m_{ap}	Var^α_{ap}	$\mathrm{Var}_{\inf}(\sigma_1^2)$
.0	.004	.004	.008	.005	.003
.1	.022	.018	.024	.019	.015
.2	.050	.043	.049	.041	.036
.5	.195	.185	.176	.161	.143
1.0	.634	.699	.566	.539	.462
2.0	2.276	2.801	2.012	1.961	1.605
5.0	11.862	12.001	11.685	11.561	9.041

Table 4.5. The results of simulations and approximations of REML estimators of σ_1^2 for the model $P_{12} = (2, 10, 18)$.

σ_1^2	$\hat{\sigma}_{1(SM)}^2$	$\hat{\sigma}_1^2$	Var_{SM}	Var_{GMU}	Var_{ap}^m	Var_{ap}^α	$\mathrm{Var}_{\inf}(\sigma_1^2)$
.0	.054	.022	.021	.031	.017	.011	.006
.1	.143	.123	.069	.080	.053	.041	.028
.2	.241	.222	.139	.147	.108	.091	.062
.5	.532	.519	.482	.514	.394	.361	.231
1.0	1.039	1.017	1.456	1.491	1.272	1.211	.714
2.0	2.046	2.021	5.160	5.193	4.525	4.411	2.433
5.0	4.973	5.038	26.650	27.610	26.289	26.011	13.588

Table 4.6. The estimated probabilities from simulations for regions of positive determinability of variance-covariance matrices Σ and Σ_0 and variance component σ_1^2 for the model $P_{12} = (2, 10, 18)$.

σ_1^2	$ML - estimation$		$REML - estimation$	
	$\hat{P}(\Sigma > 0)$	$\hat{P}(\sigma_1^2 > 0)$	$\hat{P}(\Sigma_0 > 0)$	$\hat{P}(\sigma_1^2 > 0)$
.0	.610	.343	.618	.349
.1	.739	.510	.744	.546
.2	.780	.621	.797	.639
.5	.861	.763	.868	.765
1.0	.910	.846	.914	.850
2.0	.943	.901	.949	.908
5.0	.976	.951	.979	.958

Example 3. Characteristics of design for k-pattern P_{13}=(3, 15, 27).

n	p	α_1	α_2	α_3	s_4	m_1	m_2	m	α	ν_3	s	ν
45	1	27	15	3	42	19.432	4.168	11.800	15	42	3	2

n - number of observations;
p - rank(X);
α_i - eigenvalues of matrix V;
s_4 - multiplicity of zero eigenvalue of V;
m_i - eigenvalues of BVB';
ν_3 - multiplicity of zero eigenvalue of BVB';

m, α, s, ν are determined by formulas as in Subsection 3.2.

Table 4.7. The results of simulations and approximations of ML estimators of σ_1^2 for the model $P_{13} = (3, 15, 27)$.

σ_1^2	$\hat{\sigma}_{1(SM)}^2$	$\hat{\sigma}_1^2$	E_{ap}^m	E_{ap}^α
.0	.010	.011	−.075	−.059
.1	.059	.062	−.009	.007
.2	.113	.119	.058	.074
.5	.298	.297	.258	.274
1.0	.624	.620	.591	.607
2.0	1.299	1.308	1.258	1.274
5.0	3.270	3.379	3.258	3.274

σ_1^2	Var_{SM}	Var_{GMU}	Var_{ap}^m	Var_{ap}^α	$\text{Var}_{\text{inf}}(\sigma_1^2)$
.0	.002	.003	.004	.003	.001
.1	.015	.016	.016	.013	.011
.2	.038	.030	.037	.032	.029
.5	.167	.145	.153	.143	.125
1.0	.542	.509	.524	.506	.422
2.0	2.119	2.201	1.933	1.899	1.519
5.0	12.112	12.133	11.492	11.401	8.809

Table 4.8. The results of simulations and approximations of REML estimators of σ_1^2 for the model $P_{13} = (3, 15, 27)$.

σ_1^2	$\hat{\sigma}^2_{1(SM)}$	$\hat{\sigma}_1^2$	Var_{SM}	Var_{GMU}	Var^m_{ap}	Var^α_{ap}	$\mathrm{Var}_{\inf}(\sigma_1^2)$
.0	.035	.013	.008	.013	.008	.005	.003
.1	.127	.114	.044	.049	.034	.028	.019
.2	.216	.213	.080	.092	.081	.071	.048
.5	.507	.511	.390	.405	.342	.321	.196
1.0	1.004	1.009	1.240	1.288	1.177	1.138	.644
2.0	2.024	2.016	4.810	4.879	4.347	4.271	2.289
5.0	4.983	5.030	27.560	27.706	25.855	25.671	13.227

Table 4.9. The estimated probabilities from simulations for regions of positive determinability of variance-covariance matrices Σ and Σ_0 and variance component σ_1^2 for the model $P_{13} = (3, 15, 27)$.

σ_1^2	$ML - estimation$		$REML - estimation$	
	$\hat{P}(\Sigma > 0)$	$\hat{P}(\sigma_1^2 > 0)$	$\hat{P}(\Sigma_0 > 0)$	$\hat{P}(\sigma_1^2 > 0)$
.0	.610	.339	.613	.343
.1	.761	.559	.774	.600
.2	.829	.675	.831	.680
.5	.890	.810	.896	.816
1.0	.931	.879	.937	.886
2.0	.959	.930	.966	.936
5.0	.983	.968	.985	.973

4.1. Conclusions

Note 4.2. The values of ML and REML estimators of σ_1^2 obtained from our simulations in many cases are a little smaller in comparison with the estimates taken from simulations obtained by Swallow and Monahan [17]. It is caused by the fact that we consider the natural parameter space somewhat wider than Swallow and Monahan [17] (see also Note 4.1).

The analysis of Tables 4.1, 4.2, 4.4, 4.5, 4.7, 4.8 leads to the following conclusions:

- the REML estimators have small biases with reference to ML estimators,
- taking some correction connected with a large bias of ML estimators we can state that the REML estimators are only somewhat less effective than ML estimators,
- the proposed approximations of the expectations and the variances of ML and REML estimators of σ_1^2 are for the above simulations quite good,
- the proposed approximations of the variances of ML and REML estimators of σ_1^2 and the variances obtained from simulations are very close to values: $1.5 \cdot \mathrm{Var}_{\mathrm{inf}}$ for ML estimators and $2 \cdot \mathrm{Var}_{\mathrm{inf}}$ for REML estimators.

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