On the maximum likelihood degree of linear mixed models with two variance components

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Abstract: We extend the results concerning the upper bounds for the maximum likelihood degree and the REML degree of the one-way random effects model presented in Gross et al. [Electron. J. Stat. 6 (2012), pp. 993–1016] to the case of the normal linear mixed model with two variance components. Then we prove that both parts of Conjecture 1 in the paper of Gross et al., which concerns a certain extension of the one-way random effects model, are true under fairly mild conditions.

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1. Introduction

The notion of the maximum likelihood (ML) degree of the statistical model that has rational ML equations was introduced in [1] and [7]. It can be defined as ‘the number of complex solutions to the likelihood equations when data are generic’: a data set is generic ‘if it is not a part of the null set for which the number of complex solutions is different’ (compare [5, p. 995] and [3, Chapter 2]). It may be interpreted as a measure of the computational complexity of the problem of solving the ML equations algebraically.

In the paper [3], the authors considered the ML degree of variance component models. They also introduced the notion of the restricted maximum likelihood
(REML) degree of these models. The REML estimator of the vector of variance components can be defined as its ML estimator in the appropriately modified model; the REML degree can be defined as the ML degree of this modified model. The authors of [5] computed the ML degree and the REML degree for the one-way random effects model and formulated a conjecture concerning upper bounds for the ML degree and the REML degree of its extension, in which the mean structure is more general.

In this paper, we study the linear mixed model with two variance components. We give upper bounds for the ML degree and for the REML degree of this model. As a corollary, we obtain conditions under which the part of Conjecture 1 in [5], which concerns the upper bound for the ML degree of the mentioned earlier extension of the one-way random effects model, holds, and the similar conditions for the part of the conjecture concerning the REML degree of this model. The obtained bounds reduce to those given in [3, p. 996] in the case of the one-way random effects model.

The remaining sections of the paper are organized as follows. Basic facts concerning the linear mixed model with two variance components are gathered in Section 2. The theorems giving upper bounds for the ML degree and the REML degree of this model are presented in Section 3 and in Section 4. The conditions under which the statements of the conjecture from [5] are true are discussed in Section 5. The final conclusion is presented in Section 6.

The following notation will be used: for a matrix $A$, $A'$ will denote the transpose of $A$, $A^+$ the Moore-Penrose inverse of $A$, rank($A$) the rank of $A$ and $\mathcal{M}(A)$ the space spanned by the columns of $A$. The determinant of a square matrix $A$ will be denoted by $|A|$. The notation $[A_1, A_2]$ will be used for a partitioned matrix consisting of two blocks: $A_1$ and $A_2$. The symbol $I_n$ will stand for the identity matrix of order $n$, $0_n$ for the $n$-dimensional column vector of zeros and $1_n$ for the $n$-dimensional column vector of ones.

2. Model with two variance components

Let us consider the normal linear mixed model with two variance components in which the dependent variable $Y$ is an $n \times 1$ normally distributed vector with

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

(2.1)

where $X$ is an $n \times p$ matrix of full rank, $p < n$, $\beta$ is a $p \times 1$ parameter vector, $V$ is an $n \times n$ non-negative definite symmetric non-zero matrix of rank $k < n$ and $s = (\sigma_1^2, \sigma_2^2)'$ is an unknown vector of variance components belonging to $S = \{s : \sigma_1^2 \geq 0, \sigma_2^2 > 0\}$. We will denote this model by $\mathcal{N}(Y, X\beta, \Sigma(s))$; for more information concerning this approach to representing the linear mixed models, see [8, p. 7].

The twice the log-likelihood function is given, up to an additive constant, by

$$
l_0(\beta, s, Y) := -\log |\Sigma(s)| - (Y - X\beta)'\Sigma^{-1}(s)(Y - X\beta).
$$

(2.2)
The ML estimator of \((\beta, s)\) is defined as the maximizer of \(l_0(\beta, s, Y)\) over \((\beta, s) \in \mathbb{R}^n \times S\).

Let \(M := I_n - XX^+\). It can be shown that
\[
l_0(\beta, s, Y) \leq l_0(\tilde{\beta}, s, Y) = -\log |\Sigma(s)| - Y'R(s)Y,
\]

where \(R(s) := (M\Sigma(s)M)^+\) and \(\tilde{\beta}(s) := (X'S^{-1}(s)X)^{-1}X'S^{-1}(s)Y\). It can be checked that \(l_0(\beta, s, Y) < l_0(\tilde{\beta}, s, Y)\) for \(\beta \neq \tilde{\beta}\). It can be thus seen that the problem of computing the ML estimator of \((\beta, s)\) reduces to finding the maximizer of \(l(s, Y) := -\log |\Sigma(s)| - Y'R(s)Y\) over \(s \in S\), which we will refer to as the ML estimator of \(s\), compare \([11], p. 230\) and \([4, 284]\). It can be also observed that for a given value \(y\) of the vector \(Y\) the ML estimate of \(s\) exists if and only if the ML estimate of \((\beta, s)\) exists.

It can be verified that the complex solutions to the ML equations obtained by equating \(\partial l_0(\beta, s, Y)/\partial \beta\), \(\partial l_0(\beta, s, Y)/\partial \sigma^2_1\) and \(\partial l_0(\beta, s, Y)/\partial \sigma^2_2\) to 0 (or to 0\(p\)) are of the form \((\tilde{\beta}(\hat{s}), \hat{s})\), where \(\hat{s}\) is a complex solution to the system
\[
\frac{\partial l(s, Y)}{\partial \sigma^2_1} = 0, \quad \frac{\partial l(s, Y)}{\partial \sigma^2_2} = 0. \tag{2.3}
\]

Here the partial derivatives are computed with respect to the real variables \(\sigma^2_1\), \(\sigma^2_2\) and \(\beta\). It can be also checked that if \(\hat{s}\) is a solution to (2.3), then \((\tilde{\beta}(\hat{s}), \hat{s})\) is a solution to the ML equations. The ML degree of the model (2.1) is thus equal to the number of complex solutions to the system (2.3) when the data are generic.

The necessary and sufficient condition for the existence of the ML estimate of \(s\) is given in the following

**Theorem 2.1.** For a given value \(y\) of the vector \(Y\), the ML estimate of \(s\) exists if and only if
\[
y \notin M([X, V]). \tag{2.4}
\]

**Proof.** The theorem is an immediate consequence of Theorem 3.1 in [2]. \(\square\)

**Corollary 2.1.** The ML estimate of \(s\) exists with probability 1 if and only if
\[
M([X, V]) \subseteq \mathbb{R}^n. \tag{2.5}
\]

Let \(B\) be an \((n - p) \times n\) matrix satisfying the conditions
\[
BB' = I_{n-p}, \quad B'B = M. \tag{2.6}
\]

The ML estimator of \(s\) in the model \(\mathcal{N}(z, 0_{n-p}, \sigma^2_1 BVB' + \sigma^2_2 I_{n-p})\), where \(z := BY\), is known in the literature as the restricted maximum likelihood (REML) estimator of \(s\) (compare e.g. \([4, p. 291]\) or \([10, p. 880]\)).

Let
\[
BV B' = \sum_{i=1}^{d-1} m_i E_i \tag{2.7}
\]
be the spectral decomposition of $BV B'$, where $m_1 > \ldots > m_{d-1} > m_d = 0$ denotes the decreasing sequence of distinct eigenvalues of $BV B'$ and $E_i$'s are orthogonal projectors satisfying the condition $E_i E_j = 0_{n-p}$ for $i \neq j$. Let $E_d$ be such that $\sum_{i=1}^d E_i = I_{n-p}$ and let

$$T_i := z' E_i z / \nu_i, \quad z := BY,$$

where $\nu_i$ denotes the multiplicity of the eigenvalue $m_i$, $i = 1, \ldots, d$. Let us note that the quantities $m_i$, $E_i$, and $\nu_i$, $i = 1, \ldots, d$, do not depend on the choice of $B$ in (2.6), see [10, p. 880]. Throughout the paper we will assume that $\nu_d > 0$.

The random variables $T_i$'s are mutually independent and $\nu_i (m_i \sigma_1^2 + \sigma_2^2)^{-1} T_i$ has a central chi-squared distribution with $\nu_i$ degrees of freedom, $i = 1, \ldots, d$, compare [10, p. 880].

It can be shown that

**Theorem 2.2.** For a given value $y$ of the vector $Y$ in the model (2.1), the REML estimate of $s$ exists if and only if

$$My \notin M(MV).$$

**Proof.** The theorem follows directly from Theorem 3.4 in [2].

**Proposition 2.1.** The REML estimate of $s$ in the model (2.1) exists with probability one if and only if

$$M(MV) \subseteq M(M).$$

**Proof.** It can be seen that $M(MV) \subseteq M(M)$ if and only if $M(BV) \subseteq \mathbb{R}^{n-p}$. Since $BY \sim N(0_{n-p}, \sigma_1^2 BV B' + \sigma_2^2 I_{n-p})$, we have: $P(My \notin M(MV)) = P(BY \notin M(BV)) = 1$ if and only if (2.11) holds.

**Proposition 2.2.** In the model (2.1):

(a) The condition (2.5) implies the condition (2.11).

(b) The condition (2.11) is equivalent to the condition (2.9).

**Proof.** To prove the part (a) let us assume that $M(MV) = M(M)$. This condition implies that $M(M) \subset M(V)$, which is equivalent to $M([X, V]) = \mathbb{R}^n$, and so we have obtained a contradiction.

The part (b) is a consequence of the following facts: the condition (2.11) is equivalent to $M(BV) \subset \mathbb{R}^{n-p}$ and $M(BV) = M(BV B')$.

3. The ML degree of the model

Let $\alpha_1 > \alpha_2 > \ldots > \alpha_{d_0} = 0$ denote the decreasing sequence of distinct eigenvalues of $V$ and let $s_i$, $i = 1, \ldots, d_0$, stand for their multiplicities. The ML
equation system (2.3) can be written as
\[
\sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} T_i = \sum_{j=1}^{d-1} \frac{s_j \alpha_j}{\alpha_j \sigma_1^2 + \sigma_2^2}, \\
\sum_{i=1}^{d} \frac{\nu_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} T_i = \sum_{j=1}^{d} \frac{s_j}{\alpha_j \sigma_1^2 + \sigma_2^2},
\]
(3.1)

compare [4, p. 286].

Let us introduce the variables
\[
\sigma^2 := \sigma_1^2 + \sigma_2^2, \quad \rho := \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2}.
\]

It can be seen that
\[
\sigma_1^2 = \sigma^2 \rho, \quad \sigma_2^2 = \sigma^2 (1 - \rho).
\]
(3.2)

Let us define the rational algebraic expressions
\[
\phi_\mu(\rho) := (\mu - 1) \rho + 1, \quad H_1(\rho) := \sum_{i=1}^{d-1} \frac{\nu_i m_i}{\phi_{\mu_i}(\rho)} T_i, \\
H_2(\rho) := \sum_{j=1}^{d-1} \frac{\alpha_j s_j}{\phi_{\alpha_j}(\rho)}, \quad \text{and} \quad h(\rho) := \frac{H_1(\rho)}{H_2(\rho)}.
\]
(3.3)
(3.4)

If \(T_i > 0\) for some \(i < d\), then the system (3.1), assuming that \(\sigma_1^2 + \sigma_2^2 \neq 0\), is equivalent to:
\[
\sigma^2 = h(\rho),
\]
(3.5)
\[
\sum_{i=1}^{d} \frac{\nu_i}{\phi_{\mu_i}(\rho)} T_i = h(\rho) \sum_{j=1}^{d} \frac{s_j}{\phi_{\alpha_j}(\rho)},
\]
(3.6)

compare [4, p. 287]. Let us observe that if we find a solution to (3.6) with respect to \(\rho\), we will be able to compute a solution to the system (3.1) using (3.5) and (3.2). Let us also note that each solution to (3.1) that does not have the form \((\theta, -\theta)\), where \(\theta\) is a complex number, can be obtained in this way if \(T_i > 0\) for some \(i < d\). Finding solutions to (3.6) in turn reduces to finding roots of \(P(\rho) := P_1(\rho) P_2(\rho) - P_3(\rho) P_4(\rho)\) with the polynomials \(P_1(\rho), P_2(\rho), P_3(\rho),\) and \(P_4(\rho)\) obtained by simplifying
\[
R_1(\rho) := \sum_{i=1}^{d} \frac{\nu_i}{\phi_{\mu_i}(\rho)} T_i Q_1(\rho)(1 - \rho)^2, \quad R_2(\rho) := \sum_{j=1}^{d-1} \frac{\alpha_j s_j}{\phi_{\alpha_j}(\rho)} Q_2(\rho), \\
R_3(\rho) := \sum_{i=1}^{d-1} \frac{\nu_i m_i}{\phi_{\mu_i}(\rho)} Q_1(\rho) T_i, \quad \text{and} \quad R_4(\rho) := \sum_{j=1}^{d} \frac{s_j}{\phi_{\alpha_j}(\rho)} Q_2(\rho)(1 - \rho)^2,
\]
respectively, where
\[ Q_1(\rho) := \prod_{i=1}^{d-1} \phi_{m_i}^2(\rho) \quad \text{and} \quad Q_2(\rho) := \prod_{j=1}^{d_0-1} \phi_{\alpha_j}(\rho). \]

It can be seen that if \( \phi_\tau(\rho) \neq 0 \), where \( \tau \in \{m_1, m_2, \ldots, m_d\} \cup \{s_1, s_2, \ldots, s_{d_0}\} \), and \( P(\rho) = 0 \), then \( \rho \) is a solution to the equation (3.6). Let us note that all solutions to (3.6) can be obtained in this way.

It can be shown that

**Theorem 3.1.** (a) The degree of \( P(\rho) \) is bounded from above by \( 2d + d_0 - 4 \).
(b) If the condition (2.5) holds, then \( P(\rho) \) is a non-zero polynomial with probability 1.

**Proof.** The proof easily follows from Theorem 2.5 in [6]. \( \square \)

The above theorem suggests that the ML degree of the linear mixed model with two variance components does not exceed \( 2d + d_0 - 4 \) if the appropriate assumptions are satisfied. To prove this, we need the following

**Lemma 3.1.** The probability that the ML equations (3.1) have a solution of the form \( s = (\theta, -\theta) \), where \( \theta \) belongs to the set of complex numbers, is equal to 0.

**Proof.** Upon substitution \( \theta \) for \( \sigma_{11}^2 \) and \( -\theta \) for \( \sigma_{22}^2 \) the system (3.1) reduces to the following set of equations:

\[
\begin{align*}
\sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i - 1)^2} T_i &= \theta \sum_{j=1}^{d_0-1} \frac{s_j \alpha_j}{\alpha_j - 1}, \\
\sum_{i=1}^{d} \frac{\nu_i}{(m_i - 1)^2} T_i &= \theta \sum_{j=1}^{d_0} \frac{s_j}{\alpha_j - 1}, \\
\theta &= 0.
\end{align*}
\]

(3.7)

Let us observe that if
\[
\sum_{j=1}^{d_0-1} \frac{s_j \alpha_j}{\alpha_j - 1} = 0,
\]

(3.8)

then the left-hand side of the first equation in the system (3.7) is equal to 0. This implies that \( T_i = 0, \ i = 1, 2, \ldots, d - 1 \). The probability of this event is equal to 0.

If the condition (3.8) does not hold, then
\[
\theta = \frac{\sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i - 1)^2} T_i}{\sum_{j=1}^{d_0-1} \frac{s_j \alpha_j}{\alpha_j - 1}}
\]

can be regarded as a function of \( T_1, \ldots, T_{d-1} \) and the second equation of the system (3.7) can be rewritten in the form

\[
\sum_{i=1}^{d} \frac{\nu_i}{(m_i - 1)^2} T_i - \theta \sum_{j=1}^{d_0} \frac{s_j}{\alpha_j - 1} = 0.
\]

(3.9)
The left-hand side of the above equation can be expressed as the sum of the independent random variables $X_1$ and $X_2$ given by

$$X_1 = \frac{\nu_d}{(m_d - 1)^2} T_d, \quad X_2 = \sum_{i=1}^{d-1} \frac{\nu_i}{(m_i - 1)^2} T_i - \theta \sum_{j=1}^{d_0} \frac{s_j}{\alpha_j - 1}.$$ 

Since $X_1$ is absolutely continuous, the sum $X_1 + X_2$ has a density (so it cannot have an atom in 0) and this completes the proof.

An immediate consequence of Lemma 3.1, Theorem 3.1, and the fact that $T_i > 0$ outside a null set $(i = 1, \ldots, d)$ is

**Theorem 3.2.** If the model (2.1) satisfies the condition (2.5), then its ML degree is bounded from above by $2d + d_0 - 4$.

### 4. The REML degree of the model

The REML equation system, that is the ML equation system in the model $\mathcal{N}\{z, \mathbf{0}_{n-p}, \sigma_1^2 \mathbf{B} \mathbf{V} \mathbf{B}' + \sigma_2^2 \mathbf{I}_{n-p}\}$ with $z = \mathbf{B} \mathbf{Y}$, where $\mathbf{B}$ is a matrix satisfying the condition (2.6), can be presented in the form

$$
\begin{align*}
\sum_{i=1}^{d-1} \frac{\nu_i m_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} T_i &= \sum_{j=1}^{d-1} \frac{\nu_j m_j}{m_j \sigma_1^2 + \sigma_2^2}, \\
\sum_{i=1}^{d} \frac{\nu_i}{(m_i \sigma_1^2 + \sigma_2^2)^2} T_i &= \sum_{j=1}^{d} \frac{\nu_j}{m_j \sigma_1^2 + \sigma_2^2}.
\end{align*}
$$

(4.1)

see [4, p. 291]. If $T_i > 0$ for some $i < d$, then finding all the solutions to the system (4.1) that don’t have the form $s = (\theta, -\theta)'$, where $\theta$ is a complex number, can be reduced to finding all roots of the polynomial $P^*(\rho)$ obtained by simplifying the algebraic expression

$$
P^*_0(\rho) := (R^*_1(\rho) - R^*_2(\rho))Q^*_1(\rho),
$$

where

$$
R^*_1(\rho) := \sum_{i=1}^{d} \frac{\nu_i}{\phi_{m_i}(\rho)} T_i \sum_{j=1}^{d-1} \frac{m_j \nu_j}{\phi_{m_j}(\rho)},
$$

$$
R^*_2(\rho) := \sum_{i=1}^{d-1} \frac{\nu_i m_i}{\phi_{m_i}(\rho)} T_i \sum_{j=1}^{d} \frac{\nu_j}{\phi_{m_j}(\rho)}
$$

and

$$
Q^*_1(\rho) := \prod_{i=1}^{d} \phi_{m_i}^2(\rho)
$$

(4.3)

in a similar way as in the case of the ML equations.

**Theorem 4.1.** (a) The degree of the polynomial $P^*(\rho)$ is bounded from above by $2d - 3$.

(b) If the condition (2.11) holds, then $P^*(\rho)$ is a non-zero polynomial with probability 1.

**Proof.** The theorem easily follows from Theorem 3.1 in [6].
The REML degree of the linear mixed model $N(Y, X\beta, \Sigma(s))$ can be defined as the ML degree of the model $N(BY, 0_{n-p}, B\Sigma(s))B'$, where $B$ is a matrix satisfying (2.6).

**Theorem 4.2.** If the model (2.1) satisfies the condition (2.11), then its REML degree does not exceed $2d - 3$.

We omit the proof of Theorem 4.2 since it is similar to that of Theorem 3.2.

5. General mean structure in the one-way layout

Let us consider the following extension of the one-way random effects model:

$$Y = W\beta + Z\alpha + \epsilon,$$  \hspace{1cm} (5.1)

where $\beta \in \mathbb{R}^p$ is a fixed mean parameter vector, $\alpha = (\alpha_1, \ldots, \alpha_q)'$ with $q \geq 2$ is the vector of random effects, $W$ is an $n \times p$ matrix of rank $p < n$ such that $1_n \in \mathcal{M}(W)$ and

$$Z = \begin{bmatrix} 1_{n_1} & 0_{n_1} & \cdots & 0_{n_1} \\ 0_{n_2} & 1_{n_2} & \cdots & 0_{n_2} \\ \vdots & \vdots & \ddots & \vdots \\ 0_{n_q} & 0_{n_q} & \cdots & 1_{n_q} \end{bmatrix},$$ \hspace{1cm} (5.2)

where $n = \sum_{k=1}^{q} n_k$. We assume that $\alpha \sim N(0_q, \sigma_1^2 I_q)$ and $\epsilon \sim N(0_n, \sigma_2^2 I_n)$ are independent. The model was considered e.g. in [5, Section 5]. It can be expressed in the form (2.1) with $X = W$ and $V = ZZ'$.

To find upper bounds for the ML degree and the REML degree of this model we will need the following

**Proposition 5.1.** In the model (2.1) with $X = W$ and $V = ZZ'$:

(a) The number of distinct eigenvalues of the matrix $V$ does not exceed $q + 1$.

(b) The number of distinct eigenvalues of the matrix $BV B'$ does not exceed $q$.

**Proof.** The proof of the part (a) follows from the equalities

$$\text{rank}(V) = \text{rank}(ZZ') = \text{rank}(Z) = q.$$  

For the proof of (b) it is sufficient to note that $MVM = \sum_{i=0}^{d} m_i B'E_iB$, where $m_i$ and $E_i$, are as in (2.7), see [4, p. 285], and

$$\text{rank}(BV B') = \text{rank}(MVM) = \text{rank}(MZ) < \text{rank}(Z) = q.$$  

Now we are ready to state the following

**Theorem 5.1.** Consider the model (2.1) with $X = W$ and $V = ZZ'$.
(a) If the condition (2.5) is satisfied, then the ML degree of the model does not exceed $3q - 3$.
(b) If the condition (2.11) is satisfied, then the REML degree of the model does not exceed $2q - 3$.

Proof. The part (a) of the theorem is a consequence of Theorem 3.2 and Proposition 5.1 while the part (b) follows from Theorem 4.2 and Proposition 5.1. □

We have thus proved that both parts of Conjecture 1 in the paper of Gross et al. [5], which concerns the maximum likelihood degree and the REML degree of the model (5.1), are true under fairly mild conditions.

Remark 5.1. The condition (2.5) as well as the condition (2.11) are satisfied if $n_k > 1$ for some $k$. The above theorem can be thus considered as a generalization of the results concerning the bounds for the ML degree and the REML degree for the one-way random effects model presented in [5, p. 996].

6. Conclusion

The recent research confirms that the likelihood function and the REML likelihood function may have multiple local maxima, see e.g. [9, pp. 2296–2297] or [5, Section 7]. The results obtained in this paper indicate that the approach proposed in the paper of Gross et al. [5], in which all critical points of the log-likelihood function are found by solving a system of algebraic equations, may prove to be efficient for linear mixed models with two variance components.

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