

A dimension reduction technique for estimation in linear mixed models

M. de Carvalho^{a*}, M. Fonseca^b, M. Oliveira^c and J.T. Mexia^b

^aSwiss Federal Institute of Technology, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ^bFaculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Lisboa, Portugal; ^cColégio Luis António Verney, Universidade de Évora, Évora, Portugal

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This paper proposes a dimension reduction technique for estimation in linear mixed models. Specifically, we show that in a linear mixed model, the maximum-likelihood (ML) problem can be rewritten as a substantially simpler optimization problem which presents at least two main advantages: the number of variables in the simplified problem is lower and the search domain of the simplified problem is a compact set. Whereas the former advantage reduces the computational burden, the latter permits the use of stochastic optimization methods well qualified for closed bounded domains. The developed dimension reduction technique makes the computation of ML estimates, for fixed effects and variance components, feasible with large computational savings. Computational experience is reported here with the results evidencing an overall good performance of the proposed technique.

Keywords: maximum-likelihood estimation; linear mixed models; stochastic optimization

1. Introduction

Maximum-likelihood methods are among the main standard techniques for yielding parameter estimates for a statistical model of interest. The large sample characterization of this M -estimation methodology has long been established in the literature [1]. Despite the attractive features of maximum-likelihood (ML) procedures, in a plurality of cases of practical interest, the proposed estimators are not analytically tractable. To overcome the lack of closed-form analytic solution, global optimization methods are typically employed. This feature is *not* peculiar to ML estimation, as it is more generally shared by the broad class of extremum estimators, i.e. estimators which are motivated by an optimization problem of interest [2,3]. In this paper, we are concerned with a particular case where such an occurrence takes place, namely in the ML estimation of a linear mixed model. As we discuss below, this model is a popular extension of the linear model that is able to account for more than one source of error (see Section 2). A general overview of topics related with estimation and inference in linear mixed models can be found in [4–6].

Before conducting the estimation and inference, it is advisable to inspect if the problem at hand can be simplified analytically. Hence, for instance, as noted by Carvalho *et al.* [7,8], if the

*Corresponding author. Email: miguel.carvalho@epfl.ch

linear mixed model has a common orthogonal block structure, then a closed-form solution for the ML estimator can be found. Other than in these special instances, it is seldom possible to achieve an explicit form for the solution of this ML problem. Notwithstanding, here we show that in a linear mixed model, the ML problem can be rewritten as a much simpler optimization problem (henceforth, the simplified problem), whose size depends only on the number of variance components. The original ML formulation is thus reduced into a simplified problem which presents at least two main advantages: the number of variables is considerably lower and the search domain is compact. As it can be readily appreciated, these features are extremely advantageous from the computational standpoint. In effect, this simplified problem endows us with the means to obtain estimates of variance components with large computational savings. In addition, given that the search domain of the simplified problem is compact, we can apply stochastic optimization methods well qualified for closed bounded domains [9,10].

The remainder of this paper is structured as follows. In Section 2 we introduce the models of interest. The main result and simulation studies are presented in Section 3; final remarks are given in Section 4.

2. Models

2.1. The linear mixed model

The simple linear model is at the heart of a broad number of statistical applications. In its elementary form, the model is commonly stated as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}_0 + \boldsymbol{\epsilon}, \quad (1)$$

where \mathbf{y} is the $(n \times 1)$ vector of observations, \mathbf{X} is the design matrix of size $n \times k$, $\boldsymbol{\beta}_0$ is a $(k \times 1)$ vector of unknown regression parameters, and $\boldsymbol{\epsilon}$ is the $(n \times 1)$ vector of unobserved errors. In this paper, our interest relies on a well-known generalization of the linear model (1), namely the linear mixed model. From the conceptual stance, the model can be thought as an extension of the linear model that is qualified to consider distinct sources of error. Specifically, the linear mixed model takes the following form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}_0 + \sum_{i=1}^{w-1} \mathbf{X}_i \boldsymbol{\zeta}_i + \boldsymbol{\epsilon}, \quad (2)$$

where $(\mathbf{y}, \mathbf{X}, \boldsymbol{\beta}_0, \boldsymbol{\epsilon})$ are defined as in Equation (1), \mathbf{X}_i are design matrices of size $n \times k_i$, and where $\boldsymbol{\zeta}_i$ are the $(k_i \times 1)$ -vectors of unobserved random effects. Following classical assumptions, we take the random effects $\boldsymbol{\zeta}_i$ to be independent and normally distributed with null mean vectors and covariance matrix $\sigma_{0i}^2 \mathbf{I}_{k_i}$, for $i = 1, \dots, w-1$. Further, we also take the $\boldsymbol{\epsilon}$ to be normally distributed with a null mean vector and a covariance matrix $\sigma_{0w}^2 \mathbf{I}_n$, independently of the $\boldsymbol{\zeta}_i$, for $i = 1, \dots, w-1$. The model has the following mean vector and covariance matrix

$$E\{\mathbf{y}|\mathbf{X}\} = \mathbf{X}\boldsymbol{\beta}_0, \\ \boldsymbol{\Sigma}_{\sigma_0^2} = \sum_{i=1}^{w-1} \sigma_{0i}^2 \mathbf{X}_i \mathbf{X}_i' + \sigma_{0w}^2 \mathbf{I}_n,$$

where $\boldsymbol{\sigma}_0^2 = (\sigma_{01}^2, \dots, \sigma_{0w}^2)$. Given the current framework, we have that

$$\mathbf{y}|\mathbf{X} \sim \mathcal{N}\left(\mathbf{X}\boldsymbol{\beta}_0; \sum_{i=1}^{w-1} \sigma_{0i}^2 \mathbf{X}_i \mathbf{X}_i' + \sigma_{0w}^2 \mathbf{I}_n\right),$$

and thus the density for the model is given by

$$f_{\mathbf{y}|\mathbf{X}}(\mathbf{y}) = \frac{\exp(-(1/2)(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}_0)' \boldsymbol{\Sigma}_{\sigma_0^2}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}_0))}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}_{\sigma_0^2}|}}.$$

The estimator objective function assigned to the ML estimator is given by the log-likelihood of the aforementioned linear mixed model, i.e.

$$\mathcal{L}_n(\boldsymbol{\beta}, \sigma^2) = -\frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\boldsymbol{\Sigma}_{\sigma^2}| - \frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \boldsymbol{\Sigma}_{\sigma^2}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

The ML estimators of the true parameter $\boldsymbol{\beta}_0$ and the model variance components σ^2 , respectively, denoted by $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are thus

$$\begin{pmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\sigma}^2 \end{pmatrix} = \arg \max_{(\boldsymbol{\beta}, \sigma^2)' \in \mathbb{R}^k \times \mathbb{R}^w} \mathcal{L}_n(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}). \tag{3}$$

In the following section, we consider a special case, wherein it is possible to obtain a closed-form solution for this ML problem. It should be emphasized that cases such as those presented below represent the exception, rather than the rule, and this instance should only be regarded as a benchmark.

2.2. The benchmark case

In this section, we consider a particular case of model (2), wherein it is possible to get a closed-form solution for the problem of interest. As we shall see below, this is gained at the cost of the introduction of some structure in the covariance matrix $\boldsymbol{\Sigma}_{\sigma_0^2}$. Specifically, we consider the case wherein the covariance matrix can be decomposed as a linear combination of known orthogonal projection matrices \mathbf{Q}_j , i.e.

$$\boldsymbol{\Sigma}_{\sigma_0^2} = \sum_{j=1}^w \eta_j \mathbf{Q}_j.$$

If \mathbf{Q}_j are orthogonal projection matrices such that $\mathbf{Q}_j \mathbf{Q}_{j'} = \mathbf{0}$ for $j \neq j'$, and if \mathbf{T} , the orthogonal projection matrix on the range space of \mathbf{X} , is such that

$$\mathbf{T} \mathbf{Q}_j = \mathbf{Q}_j \mathbf{T}, \quad j = 1, \dots, w,$$

the model is said to have a commutative orthogonal block structure [11,12]. Here, $\boldsymbol{\eta} = (\eta_1, \dots, \eta_w)'$ is the vector of the so-called canonical variance components and it is determined by the equation $\mathbf{B}\boldsymbol{\eta} = \boldsymbol{\sigma}_0^2$, where \mathbf{B} is a known nonsingular matrix. In this case, we can rewrite the density of the model as

$$f_{\mathbf{y}|\mathbf{X}}(\mathbf{y}) = \frac{\exp(-(1/2)(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}_0)' (\sum_{j=1}^w \eta_j^{-1} \mathbf{Q}_j) (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}_0))}{\sqrt{(2\pi)^n \prod_{j=1}^w \eta_j^{g_j}}},$$

where g_j is the rank of matrix \mathbf{Q}_j [11, Theorem 1]. In this particular instance, it can be shown [7] that the estimators

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y}$$

and

$$\hat{\eta}_j = \frac{\mathbf{y}'(\mathbf{I} - \mathbf{T})\mathbf{Q}_j(\mathbf{I} - \mathbf{T})\mathbf{y}}{g_j}$$

solve the optimization problem (3).

When the above-mentioned conditions on the covariance matrix do not hold, a closed-form analytical expression for producing ML estimates is hardly available.

3. Main result and simulation study

3.1. Main result

The next result establishes that in a linear mixed model, the ML problem can be rewritten as a simplified problem where the search domain is a compact set whose dimension depends exclusively on the number of variance components. This result will be useful to compute the estimation of variance components, through ML methods, with the application of random search methods.

THEOREM 1 *The ML estimators of the true parameter β_0 , and the model variance components σ_0^2 , respectively, denoted by $\hat{\beta}$ and $\hat{\sigma}^2$*

$$\begin{pmatrix} \hat{\beta} \\ \hat{\sigma}^2 \end{pmatrix} = \arg \max_{(\beta, \sigma^2) \in \mathbb{R}^k \times \mathbb{R}^w} \mathcal{L}_n(\beta, \sigma^2 | \mathbf{y}),$$

can be alternatively achieved by solving the following optimization problem

$$\min_{\boldsymbol{\gamma} \in [0, \pi/2]^{w-1}} (f_n \circ \mathbf{p})(\boldsymbol{\gamma}),$$

where

$$f_n(\boldsymbol{\alpha}) = \ln(A(\boldsymbol{\alpha})^n | \boldsymbol{\Sigma}_{\boldsymbol{\alpha}}), \quad (4)$$

$$A(\boldsymbol{\alpha}) = \mathbf{y}'(\mathbf{I} - \mathbf{X}(\mathbf{X}'\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}^{-1}\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}^{-1})'\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}^{-1}(\mathbf{I} - \mathbf{X}(\mathbf{X}'\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}^{-1}\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}^{-1})\mathbf{y}, \quad (5)$$

$$\mathbf{p}(\boldsymbol{\gamma}) = \mathbf{e}_1 \prod_{j=1}^{w-1} \cos(\gamma_j) + \sum_{l=2}^{w-1} \mathbf{e}_l \left(\prod_{j=1}^{w-l} \cos(\gamma_j) \sin(\gamma_{w-l}) \right) + \mathbf{e}_w \sin(\gamma_{w-1}), \quad (6)$$

and $\{\mathbf{e}_i\}_{i=1}^w$ denotes the canonical basis of \mathbb{R}^w .

As discussed above, we can ascertain at least two major advantages of the simplified problem, viz.

- whereas the original ML problem has dimension $(w + k)$, the simplified equivalent problem only has size $(w - 1)$; additionally,
- the search domain of the simplified problem is $[0; \pi/2]^{w-1}$, and hence is compact (contrarily to what is verified in the original problem).

The proof is given in the appendix.

3.2. A first Monte Carlo simulation study

In this simulation study, we considered three one-way random models. (This study was implemented in R. The code is available from the authors.) The first model is unbalanced with a total of 72 observations and 8 groups; the arrangement of the observations is described in Table 1. Several possible true values of the variance components are considered below.

We then conducted a Monte Carlo simulation from which we report the averaging of the 1000 results achieved. In every run of the simulation, the optimization problem was solved by combining a random search technique with the dimension reduction technique introduced in Section 3.1. The random search algorithm used as input 10,000 evaluations of the objective function of the simplified problem. Hence, 10,000 values of $\boldsymbol{\gamma} \in [0; \pi/2]$ were randomly selected and their corresponding images were generated via $(f_n \circ \mathbf{p})$.

We now provide some guidelines to the interpretation of Table 2. In the first line, we present the true values of the variance components σ_{01}^2 . The second line includes the solution provided by the recurrent application of random search methods to the optimization problem (3). Thus, for instance, when the ‘true’ variance component was 0.5, the result yield through the application of stochastic optimization methods and the dimension reduction method is 0.425. Further, observe that, except when the true value of the variance component is null, the true values always dominate the estimated values.

Next, we considered a quasi-balanced model with 66 observations; the disposal of the observations was now given according to Table 3. A Monte Carlo simulation was once more conducted. No changes were made to the true values of the variance components considered. The same applies to the methods used to perform the optimization step. The produced results are reported in Table 4.

Thus, for instance, when the true value of the variance component was 0.5, the estimate obtained was now 0.448. Again, it should be emphasized that, with the exception of the case in which the true value of the variance component was 0, in all the remainder the true value was above the corresponding estimate.

A final model was then considered. The number of observations considered was now 72; observations were grouped as described in Table 5 and the results are summarized in Table 6.

Table 1. Description of the first one-way model considered (Model I).

| Group | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|--------------|---|---|---|---|---|----|----|----|
| Observations | 3 | 6 | 7 | 8 | 9 | 10 | 11 | 18 |

Notes: The model is unbalanced with 72 observations segregated over 8 groups.

Table 2. Estimates of the variance components in Model I.

| Variance component | 0.00 | 0.10 | 0.50 | 0.70 | 1.00 | 1.50 | 2.00 | 5.00 | 10.00 |
|--------------------|------|------|------|------|------|------|------|------|-------|
| Estimate | 0.02 | 0.07 | 0.43 | 0.61 | 0.87 | 1.31 | 1.76 | 4.66 | 9.42 |

Table 3. Description of the second one-way model considered (Model II).

| Group | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|--------------|---|---|---|---|---|---|---|---|---|----|----|
| Observations | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 5 | 7 |

Notes: The model is quasi-balanced with 66 observations segregated over 11 groups.

Table 4. Estimates of the variance components in Model II.

| Variance component | 0.00 | 0.10 | 0.50 | 0.70 | 1.00 | 1.50 | 2.00 | 5.00 | 10.00 |
|--------------------|------|------|------|------|------|------|------|------|-------|
| Estimate | 0.02 | 0.09 | 0.45 | 0.63 | 0.89 | 1.34 | 1.85 | 4.61 | 9.09 |

Table 5. Description of the third one-way model considered (Model III).

| Group | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|--------------|---|---|---|---|---|---|----|----|----|
| Observations | 2 | 2 | 3 | 3 | 4 | 4 | 15 | 15 | 24 |

Notes: The model is unbalanced with 72 observations segregated over 9 groups.

Table 6. Estimates of the variance components in Model III.

| Variance component | 0.00 | 0.10 | 0.50 | 0.70 | 1.00 | 1.50 | 2.00 | 5.00 | 10.00 |
|--------------------|------|------|------|------|------|------|------|------|-------|
| Estimate | 0.01 | 0.07 | 0.43 | 0.60 | 0.85 | 1.36 | 1.78 | 4.71 | 9.93 |

Table 7. Results from the second Monte Carlo simulation study.

| Variance component | 0.10 | 0.50 | 0.75 | 1.00 | 2.00 | 5.00 |
|--------------------|------|------|------|------|------|------|
| Estimate | 0.10 | 0.51 | 0.77 | 0.98 | 1.93 | 4.84 |
| RMSE | 0.06 | 0.25 | 0.39 | 0.46 | 0.80 | 2.10 |
| AAE | 0.05 | 0.19 | 0.31 | 0.36 | 0.62 | 1.69 |

As it can be readily noted from the inspection of Tables 1–3, there is a sustained bias present in the estimates, but this conforms with the existing literature; other methods, such as restricted ML, can be used to compensate for such bias [4,13].

3.3. A second Monte Carlo simulation study

In this section we report the results of a second Monte Carlo experiment. Here, a linear mixed model was considered with the following features: the fixed-effects design matrix is of size ($n = 60 \times k = 9$); the random-effects design matrix is of size ($n = 60 \times k_1 = 12$); both the fixed-effects and the random-effects matrices were randomly generated from a standard normal distribution. (This simulation study was implemented in Matlab. The routines are available from the authors upon request.) This study provides a supplement for the application of the method based on Theorem 1.

In a way similar to the previous simulation study, the application of random search entailed the collection of 10,000 sample points from the domain of the objective function ($f_n \circ \mathbf{p}$). Given the obvious increase in the burden of computation, in this section, we reduced the number of runs to 100. The true values of the variance components considered here were as follows: 0.1, 0.5, 0.75, 1, 2, 5. The results are summarized in Table 7. Here, we also include the root mean square error (RMSE) and the average absolute error (AAE) of the estimates obtained in the several runs.

4. Summary

A dimension reduction technique was proposed and applied to achieve ML estimates for the mixed model parameters and the variance components with large computational savings. The original ML problem is thus reduced into a simplified problem which presents considerable computational advantages. To illustrate the mechanics of the proposed method, two Monte Carlo simulations studies were conducted here.

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Appendix

Proof of Theorem 1 Consider the log-likelihood of the aforementioned linear mixed model,

$$\mathcal{L}_n(\boldsymbol{\beta}, \boldsymbol{\sigma}^2 | \mathbf{y}) = -\frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\boldsymbol{\Sigma}_{\sigma^2}| - \frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \boldsymbol{\Sigma}_{\sigma^2}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

Observe that maximizing $\mathcal{L}_n(\boldsymbol{\beta}, \boldsymbol{\sigma}^2 | \mathbf{y})$ is equivalent to minimizing

$$\mathcal{L}_*(\boldsymbol{\beta}, \boldsymbol{\sigma}^2 | \mathbf{y}) = \ln |\boldsymbol{\Sigma}_{\sigma^2}| + (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \boldsymbol{\Sigma}_{\sigma^2}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}). \quad (\text{A1})$$

Now define $\boldsymbol{\sigma}^2 = c\boldsymbol{\alpha}$, with $c > 0$ and $\|\boldsymbol{\alpha}\| = 1$. Making use of the first-order conditions of the ML problem, we get

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}' \boldsymbol{\Sigma}_{\sigma^2}^{-1} \mathbf{X})^{-1} \mathbf{X}' \boldsymbol{\Sigma}_{\sigma^2}^{-1} \mathbf{y}.$$

Hence, we can rewrite (A1), evaluated at $\hat{\boldsymbol{\beta}}$, as

$$\mathcal{L}_* = n \ln(c) + \ln |\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}| + c^{-1} A(\boldsymbol{\alpha}),$$

where A is defined in (5). Now, observe that

$$\frac{\partial \mathcal{L}_*}{\partial c} = nc^{-1} - c^{-2} A(\boldsymbol{\alpha}) = 0 \iff c = \frac{A(\boldsymbol{\alpha})}{n}$$

and

$$\frac{\partial^2 \mathcal{L}_*}{\partial c^2} = 2c^{-3} A(\boldsymbol{\alpha}) - nc^{-2},$$

so that

$$\left. \frac{\partial^2 \mathcal{L}_*}{\partial c^2} \right|_{c=A(\boldsymbol{\alpha})/n} = \frac{n^3}{A(\boldsymbol{\alpha})} > 0,$$

whence

$$\hat{c} = \frac{A(\boldsymbol{\alpha})}{n}$$

is an absolute minimum. Hence, Equation (A1) simplifies into $n \ln(A(\boldsymbol{\alpha})) + \ln |\boldsymbol{\Sigma}_{\boldsymbol{\alpha}}|$, which we define as $f_n(\boldsymbol{\alpha})$ (see (4)). Next, we transform $\boldsymbol{\alpha}$ through the pseudo-polar coordinate transformation $\mathbf{p}(\boldsymbol{\gamma})$, as defined in (6); further details about this

mapping can be found in [14]. This entails writing the w components of α , through $(w - 1)$ components in γ , as follows

$$\alpha_1 = \cos(\gamma_1) \cdots \cos(\gamma_{w-2}) \cos(\gamma_{w-1}),$$

$$\alpha_2 = \cos(\gamma_1) \cdots \cos(\gamma_{w-2}) \sin(\gamma_{w-1}),$$

$$\vdots$$

$$\alpha_w = \sin(\gamma_{w-1}).$$

