On the Derivation of Complex Linear Models from Simpler Ones

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Abstract

Linear mixed models are useful in biology, genetics, medical research, agriculture, industry, and many other fields, providing a flexible approach in situations of correlated data.
Based on the structure of the variance-covariance matrix, emerged a special class of linear mixed models, those of models with orthogonal block structure, which allows optimal estimation for variance components of blocks and contrasts of treatments. This approach triggered a more restrict class of mixed models, models with commutative orthogonal block structure, whose interest lies in the possibility of achieving least squares estimators giving best linear unbiased estimators for estimable vectors.
Exploring the possibility of joint analysis of linear mixed models, obtained independently, and focusing on the approach based on the algebraic structure of the models, some authors have investigated the conditions in which the good properties of the estimators are preserved.
In this work we intend to highlight the ideas underlying the techniques for the joint analysis of models, since these aspects were under-explored in the works where the theoretical formulation of the techniques were introduced. Given that these techniques were developed involving models with commutative orthogonal block structure, we provide a selective review of the literature focusing on the contributions addressing this special class of mixed linear models.

Keywords
Commutative orthogonal block structure, models crossing, models nesting, models joining.

1. Introduction

Linear models are important tools in statistical practice for analysing relationships between variables and uncover explanatory and predictive patterns. The most general formulation of linear models corresponds to linear mixed models. These models are useful in biology, genetics, medical research, agriculture, industry, and many other fields, providing a flexible approach in situations of correlated data, from, for example, repeated measurements. Addressing the accuracy of the estimators of linear mixed models, more specific classes of these models have been studied, leading to optimal estimation for variance components of blocks and contrasts of treatments, and best linear unbiased estimators for estimable vectors.

Exploring the possibility of joint analysis of several models, works emerged introducing operations between models, based on their algebraic structure (Mexia et al., 2010, Santos et al., 2017). Since, in these works, the ideas underlying the techniques for the joint analysis of models are not explicit, we believe the presentation of founding ideas can contribute to a more detailed understanding of these techniques. Given that the operations were developed involving models with commutative orthogonal block structure, we think it is opportune to carry out a selective review of the literature on this class of mixed linear models.

2. Commutative Jordan Algebras of Symmetric Matrices

Since the approach adopted for the study of the models is based on their algebraic structure, we present some notes on Commutative Jordan algebras of symmetric matrices (CJAS).

The structures known as Jordan Algebras (JA) were introduced by Jordan et al. (1934) in a reformulation of Quantum Mechanics. Rediscovered later, JA were used in statistical inference and estimation, see Seely (1970a, 1970b, 1971, 1977), Seely & Zyskind (1971). JA were also used by Michalski & Zmyślony (1996, 1999) in hypothesis test, first for variance components and later for linear combinations of parameters in mixed linear models. Many other authors have used JA (e.g. Drygas 1983, Carvalho et al. 2009). For a deeper study of Jordan algebras see, for instance, Jacobson (1968).

A Jordan algebra A is a linear space equipped with a binary operation, $\cdot$, called product, for which the following properties are verified:

- Commutative law: $a \cdot b = b \cdot a$
- Jordan identity: $(a \cdot b) \cdot a^2 = a \cdot (b \cdot a^2)$, where $a^2 = a \cdot a$

Commutative Jordan algebras of symmetric matrices (CJAS) are linear spaces constituted by symmetric matrices that commute and contain the squares of their matrices (Seely, 1971). Every CJAS has one and only one unique basis, its principal basis, constituted by pairwise orthogonal orthogonal projection matrices (POOPM). Inversely every family of POOPM is the principal basis of a CJAS (Seely 1971).

3. Classes of Linear Mixed Models

Let us consider an experiment consisting of n random observations of a response variable Y, being the response variable at the i-th of n levels expressed by

$$Y_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_k x_{ik} + \varepsilon_i \ , \ i = 1, \dots, n.$$

where $x_1, x_2, \dots, x_k$ are explanatory variables (also called regression variables, independent variables or covariates) each one with n levels, $x_{i,j}$ represents the i-th level of the j-th explanatory variable x_j, $j = 1, \dots, k$, the β_i are unknown parameters and $\underline{\varepsilon}$ is the errors vector. Rewriting the model as

$$Y_i = [x_{i0}, x_{i1}, \dots, x_{ik}] \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \varepsilon_i, \; i = 1, \dots, n ,$$

and collecting these n equations, the model can be presented in matrix notation by

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

where

$$\boldsymbol{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}$$

is the vector of observations,

$$X = \begin{bmatrix} x_{10} & x_{11} & x_{12} & \dots & x_{1k} \\ x_{20} & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ x_{n0} & x_{n1} & x_{n2} & \dots & x_{nk} \end{bmatrix}$$

is the $n \times (k+1)$ design matrix of the levels of the explanatory variables,

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

is the vector of unknown parameters, $\beta_j, j = 1, \dots, k,$ and

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

is the errors vector, which is assumed to have null mean vector and variance-covariance matrix $\sigma^2 V$, with V a known matrix and σ^2unknown.

Traditionally, linear models have been associated with fixed effect but there are several situations in which it is advantageous to incorporate the amount of variations caused by uncontrollable sources, and it is necessary to include more random effects in the model, besides the error term.

Depending on the nature of the parameters $\beta_0, \beta_1, \dots, \beta_k$, linear models are classified in three categories:

- fixed effects models: when the parameters are assumed to be constants (fixed);
- random effects models: when the parameters are random variables;
- mixed effects models: when some parameters are fixed, and others are random.

Let us consider a mixed effects linear model, or in a more abbreviated form, a linear mixed model

$$\boldsymbol{Y} = \sum_{i=0}^{w} \boldsymbol{X}_i \boldsymbol{\beta}_i$$

where $\boldsymbol{\beta}_0$ is fixed and $\boldsymbol{\beta}_1$, ... , $\boldsymbol{\beta}_w$ are independent random vectors with null mean vectors, variance-covariance matrices $\sigma_1^2 \boldsymbol{I}_{c_1} \dots \sigma_w^2 \boldsymbol{I}_{c_w}$, where $c_i = rank(\boldsymbol{X_i})$, $i = 1, \dots, w$. The matrices $\boldsymbol{X}_1, \cdots, \boldsymbol{X}_w$ are known and such that $R([\boldsymbol{X}_1 \quad \cdots \quad \boldsymbol{X}_w]) = \mathbb{R}^n$.

The model $\boldsymbol{Y}$ has mean vector

$$\boldsymbol{\mu} = \boldsymbol{X}_0 \boldsymbol{\beta}_0$$

and variance-covariance matrix

$$\boldsymbol{V} = \sum_{i=1}^{w} \sigma_i^2 \boldsymbol{M}_i, \text{ where } \boldsymbol{M}_i = \boldsymbol{X}_i \boldsymbol{X}_i^T, i = 1, \dots, w.$$

The space, Ω, spanned by $\boldsymbol{\mu}$ will be $R(\boldsymbol{X}_0)$, so the orthogonal projection matrix on Ω will be

$$\boldsymbol{T} = \boldsymbol{X}_0 (\boldsymbol{X}_0^T \boldsymbol{X}_0)^+ \boldsymbol{X}_0^T = \boldsymbol{X}_0 \boldsymbol{X}_0^+ ,$$

where the symbol + denotes the Moore-Penrose inverse of the matrix.

When the matrices $\boldsymbol{M}_1 \dots \boldsymbol{M}_w$ commute, they generate a commutative Jordan algebra of symmetric matrices (CJAS), A^0, whose principal basis is constituted by pairwise orthogonal orthogonal projection matrices (POOPM), $\boldsymbol{Q}_i^0$, $i = 1, \dots, m^0$ (Seely, 1971).

Putting

$$\boldsymbol{M_i} = \sum_{j=1}^{m^0} b_{i,j}^0 \boldsymbol{Q}_j^0 , \; i = 1, \dots, w,$$

the variance-covariance matrix, $\boldsymbol{V}$, can be written as the linear combination

$$\boldsymbol{V} = \sum_{j=1}^{m^0} \gamma_j^0 \boldsymbol{Q}_j^0,$$

with $\gamma_j^0 = \sum_{i=1}^{w} b_{i,j}^0 \sigma_i^2$, $j = 1, \dots, m^0$, the canonical variance components.

When the matrices $\boldsymbol{Q}_1^0, \dots, \boldsymbol{Q}_{m^0}^0$ add up to the identity matrix, $\sum_{j=1}^{m^0} \boldsymbol{Q}_j^0 = I_n$, the model $\boldsymbol{Y}$ belongs to a particular class of mixed models, those of models with orthogonal block structure, OBS. OBS were introduced by Nelder (1965 a, b), in the framework of the design of experiments in agricultural trials, and took on a central part in the theory of randomized block designs, see Calinski & Kageyama (2000, 2003).

Although OBS allows optimal estimation for variance components of blocks and contrasts of treatments, inference in OBS usually involves orthogonal projections on the range spaces of the matrices $\boldsymbol{Q}_j^0, j = 1, \dots, m$, which is somewhat complex due to the combination of estimators obtained from different projections. Fortunately we can overcome the difficulty associated with orthogonal projections, and achieve least squares estimators (LSE) giving best linear unbiased estimators (BLUE) for estimable vectors, focusing on a more specific class of mixed models (models with commutative orthogonal block structure - COBS), introduced by Fonseca et al. (2008).

A mixed model is COBS if it is OBS and, moreover, the orthogonal projection matrix on the space spanned by the mean vector, $\boldsymbol{T}$, commutes with the matrices $\boldsymbol{Q}_1^0, \dots, \boldsymbol{Q}_{m^0}^0$,

$$\boldsymbol{T}\boldsymbol{Q}_j^0 = \boldsymbol{Q}_j^0\boldsymbol{T}, \;\; j = 1, \dots, m^0.$$

Regarding estimation in COBS, a necessary and sufficient condition for its LSE to be BLUE is that $\boldsymbol{T}$ commutes with the variance-covariance matrix, $\boldsymbol{V}$ (Zmyślony, 1978). As shown by Fonseca et al. (2008), this commutativity condition occurs when $\boldsymbol{T}$ commutes with the matrices $\boldsymbol{Q}_1^0, \dots, \boldsymbol{Q}_{m^0}^0$. In a different approach, Santos et al. (2020) introduced a general condition for the commutativity between $\boldsymbol{T}$ and $\boldsymbol{V}$, using the fundamental partition of $\boldsymbol{Y}$ (Santos et al. 2008), constituted by the sub-vectors $\boldsymbol{Y}_1, \dots, \boldsymbol{Y}_{\dot{n}}$, corresponding to the $\dot{n}$ sets of the levels of the fixed effects factors, and resorting to U-matrices.

Following Fonseca et al. (2008), some authors continued the line of research on COBS. Santos et al. (2008) considered two successively more restrict classes of OBS and explored the possibility of completing COBS to obtain models associated to commutative Jordan algebras and truncating associated models to obtain COBS. Assuming normality, Mexia et al. (2008) obtained complete sufficient statistics for the models in a structured family of COBS. Using complete sufficient statistics, Nunes et al. (2008) got confidence regions and tests of hypotheses for variance components and estimable vectors. Carvalho et al. (2008), presented the canonic formulation of COBS, using it to carry out inference, assuming normality. Inference for structured families of segregated COBS and matching COBS was carried out by Carvalho et al. (2010). Addressing the estimation of the relevant parameters, Carvalho et al. (2011) highlighted the relevance of the fundamental partition in COBS. the relationship between COBS and error orthogonal models was explored by Carvalho et al. (2013). Ferreira (2013), discussed matching and segregation for the estimation of variance components, presenting examples in which segregation can be applied without matching. Carvalho et al. (2015) considered inference for single COBS and the joint analysis of structured families where regressions are replaced by COBS. As we will see in more detail below, Mexia et al. (2010) and Santos et al. (2017) proposed operations that allow the construction of complex models from simpler ones, enabling the joint analysis of these models.

4. Deriving Complex Models from Simpler Ones

The two most common building blocks in experimental designs are crossed factors and nested factors.

Let us consider a model with two factors. These factors are crossed when every level of one factor occurs with every level of the other factor, thus the treatments are formed as the combinations of all levels of the two factors. If we have a model with u factors, with $a_1, \dots, a_u$ levels, combining each one of the a_1 levels of the first factor with the a_2 levels of the second factor, and these a_2 levels with the a_3 levels of the third factor and so on until the a_u levels of the u-th factor, we are dealing with crossed factors and we obtain $c = \prod_{i=1}^{u} a_i$ treatments.

Let us now consider the case when there is a model whose factors are nested. We say that one factor is nested within another when any given level of the nested factor appears at only one level of the nesting factor, this is, when the levels of the nested factor are divided among the levels of the nesting factor. If we have a model with u factors, with $c_1, \dots, c_u$ levels, respectively, we have balanced nesting when the c_i , $i = 2, \dots, u$, levels of a factor are divided evenly for the c_{i-1} , $i = 2, \dots, u$, levels of the preceding factor, in groups of a_i levels. This way, the number of treatments of balanced nested models is the product of the number of the levels of the factors, $\prod_{i=1}^{u} a_i$.

In an analogy with the crossing and nesting of factors in a single model, considering several models we can perform crossing or nesting with those models.

When considering u models, each one with only one factor with $a_1, \dots, a_u$ levels, if we cross these models we obtain the same combination of levels we would have in a single model with u crossed factors, with $a_1, \dots, a_u$ levels, thus the same number of treatments. Based on this principle, the operation of Models Crossing is defined. Analogously to what was done for crossing, nesting u factors of a single model is equivalent to nesting u models, each one with only one factor. Based on this principle, the operation of Models Nesting is defined. Generalizing, we can cross or nest several models, each one of them with more than one factor.

An example of the analogy between crossed factors and Models Crossing can be seen in the following schematic representations.

In figure 1 we consider the crossing of three factors, $u = 3$, with $a_1 = 2$, $a_2 = 2$ and $a_3 = 4$ levels, respectively.

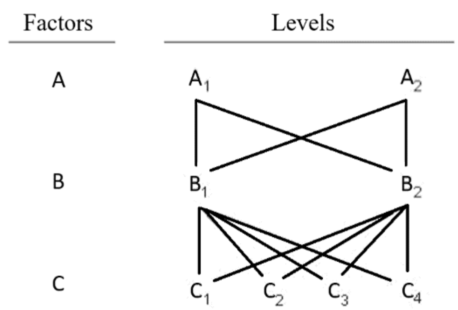

Figure 1: Factors crossing

The total number of treatments will be $c = 16$.
The same 16 treatments are obtained if we cross 3 models, each one with only one factor with $a_1 = 2$, $a_2 = 2$ and $a_3 = 4$ levels respectively, as can be seen in the schematic representation in figure 2.

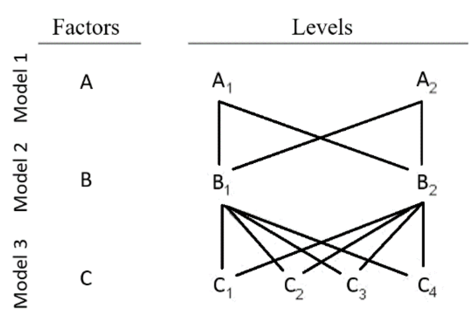

Figure 2: Model Crossing

The analogy between nested factors and Models Nesting can be seen in the following schematic representations. In figure 3 is a schematic representation of an example of balanced nesting of three factors, $u = 3$, with $c_1 = 2$, $c_2 = 6$ and $c_3 = 12$ levels, respectively.

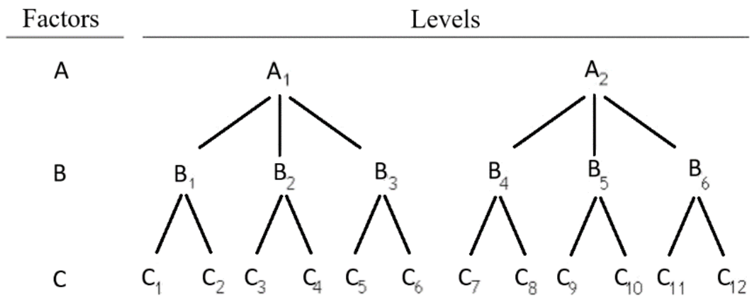

Figure 3: Factors balanced nesting

Looking at the schematic representation in figure 4, the similarity with the previous situation is evident. In this case we nest 3 models, each one with only one factor, with $c_1 = 2$, $c_2 = 6$ and $c_3 = 12$ levels, respectively

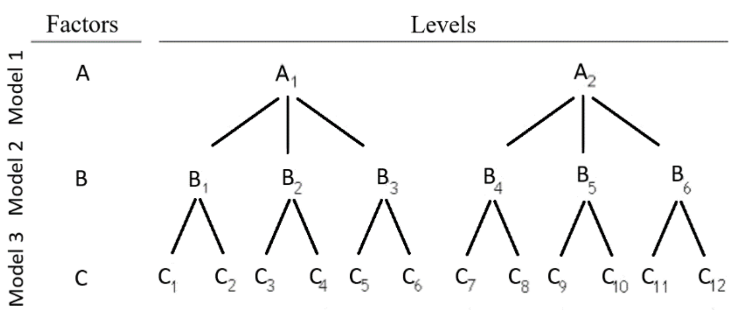

Figure 4: Model balanced nesting

The study of operations with models, using JA, was introduced by Fonseca et al. (2006). Starting from two binary operations defined on JA, more exactly on their principal basis, and taking into account that each JA is associated with an orthogonal model, Fonseca et al. (2006) considered that the binary operations defined on JA act on models, originating new models. After Fonseca et al. (2006), new developments have emerged on operations with models, extending the theory to other classes of models. Examples of this are the works of Mexia et al. (2010), that studied Model Crossing and Model Nesting, considering CCOBS and fixed effects models and Ramos et al. (2015) that studied Model Nesting, considering mixed models and fixed effects models.

As an alternative to the operations of Models Crossing and Models Nesting, Santos et al. (2017) introduced another operation, Models Joining, based on the Cartesian product of CJAS.

Following Santos et al. (2017), let us consider h mixed models

$$\boldsymbol{Y}(l) = \sum_{i=0}^{w(l)} \boldsymbol{X}_i(l)\boldsymbol{\beta}_i(l) \quad , \ l = 1, \dots, h$$

where the $\boldsymbol{\beta}_0(l)$, l = 1, ..., h, are fixed and the $\boldsymbol{\beta}_i(l)$, $i = 1, \dots, w(l)$, $l = 1, \dots, h$, have null mean vector and variance-covariance matrices $\sigma_i^2(l)I_{C_i(l)}$, $i = 1, \dots, w(l)$, $l = 1, \dots, h$, $C_i(l) = rank\left(\boldsymbol{X}_i(l)\right)$, with observations vectors

$$\boldsymbol{Y}(1) = \begin{bmatrix} Y_1(1) \\ \vdots \\ Y_{w(1)}(1) \end{bmatrix}, \quad \boldsymbol{Y}(2) = \begin{bmatrix} Y_1(2) \\ \vdots \\ Y_{w(2)}(2) \end{bmatrix}, \dots, \boldsymbol{Y}(h) = \begin{bmatrix} Y_1(h) \\ \vdots \\ Y_{w(h)}(h) \end{bmatrix}.$$

When we join these h initial models, by the superposition of the observations vectors, we obtain the observations vector

$$\boldsymbol{Y} = \begin{bmatrix} \boldsymbol{Y}_1(1) \\ \vdots \\ \boldsymbol{Y}_{w(1)}(1) \\ \boldsymbol{Y}_1(2) \\ \vdots \\ \boldsymbol{Y}_{w(2)}(2) \\ \vdots \\ \boldsymbol{Y}_1(h) \\ \vdots \\ \boldsymbol{Y}_{w(h)}(h) \end{bmatrix} = [\boldsymbol{Y}(1)^T \ \dots \ \boldsymbol{Y}(h)^T]^T .$$

So, the joint model will be

$$\boldsymbol{Y} = \sum_{i=0}^{w} \boldsymbol{X}_i \boldsymbol{\beta}_i$$

Assuming that the initial models are COBS with $w(l)$ observations, $l = 1, \dots, h$, the principal basis of the CJAS, $A(l)$, $l = 1, \dots, h$, associated to these models will be

$$\boldsymbol{Q}(l) = \left\{Q_1(l), \dots, Q_{w(l)}(l)\right\}, = 1, \dots, h$$

and the orthogonal projection matrices on the space spanned by the mean values will be

$$\boldsymbol{T}(l) = \sum_{j=1}^{w(l)} \boldsymbol{Q}_j(l) \quad , l = 1, \dots, h$$

where $\boldsymbol{T}(l) = \boldsymbol{X}_0(l)\boldsymbol{X}_0{}^T(l)$, $l = 1, \dots, h$.

Santos et al. (2017) showed that for the joint model, the principal basis of the CJAS, $\times_{i=1}^{h} A(l)$, $l = 1, \dots, h$, that is the Cartesian product of the CJAS $A(1), \dots, A(l)$, is formed by block diagonal matrices, with a single non-null block, which being the i-th block belongs to the i-th CJAS. The orthogonal projection matrix on the range space of $\boldsymbol{X}_0 = D\left(\boldsymbol{X}_0(1) \dots \boldsymbol{X}_0(h)\right)$ will be

$$\boldsymbol{T} = D\left(\boldsymbol{T}(1) \dots \boldsymbol{T}(h)\right).$$

and that

$$\boldsymbol{T}\boldsymbol{Q}_j = \boldsymbol{Q}_j\boldsymbol{T} \,,$$

concluding that joining COBS gives COBS.

Once COBS have LSE that are UBLUE (VanLeeuwen 1998), the generation of COBS from the joining of COBS is of great relevance since the good properties of the estimators are maintained.

5. Conclusion

When dealing with mixed models we may be interested in performing the joint analysis of models obtained independently. Using an approach based on the algebraic structure of the models and binary operations on Jordan Algebras two techniques have emerged to obtain complex models from simpler models: Models Crossing and Models Nesting. As an alternative to these techniques, with a similar approach, came the operation of Models Joining, which is associated to the Cartesian product of Jordan Algebras. Models with commutative orthogonal block structure (COBS) are a special class within linear mixed models. Since COBS have least squares estimators (LSE) giving best linear unbiased estimators (BLUE) for estimable vectors, it is relevant the possibility to analyse together models obtained independently.

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