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Models with commutative orthogonal block structure: a general condition for commutativity

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ABSTRACT

A linear mixed model whose variance-covariance matrix is a linear combination of known pairwise orthogonal projection matrices that add to the identity matrix, is a model with orthogonal block structure (OBS). OBS have estimators with good behavior for estimable vectors and variance components, moreover it may be interesting that the least squares estimators give the best linear unbiased estimators, for estimable vectors. We can achieve it, requiring commutativity between the orthogonal projection matrix, on the space spanned by the mean vector, and the orthogonal projection matrices involved in the expression of the variance-covariance matrix. This commutativity condition defines a more restrict class of OBS, named COBS (model with commutative orthogonal block structure). With this work we aim to present a commutativity condition, resorting to a special class of matrices, named U-matrices.

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U-matrices; best linear unbiased estimators; mixed models: models with commutative orthogonal block structure

1. Introduction

Linear mixed models play an important role in the design and analysis of experiments and have a wide use in several fields.

In the framework of the design of experiments in agricultural trials, Nelder [13,14] introduced models with orthogonal block structure (OBS), which are linear mixed models whose variance-covariance matrix is a linear combination of known pairwise orthogonal projection matrices (POPM) that add up to the identity matrix. OBS continue to play a central part in the theory of randomized block designs, (see [2,3]), which highlights the interest on the adequacy of the estimators, see e.g. [1,6].

OBS allow optimal estimation for variance components of blocks and contrasts of treatments [8] moreover we may be interested in that least squares estimators (LSE), giving best linear unbiased estimators (BLUE), for estimable vectors. For this purpose, we must impose a commutativity condition on OBS, as it was done in Fonseca et al. [10] when introducing models with commutative orthogonal block structure (COBS). COBS has been the subject of extensive research, addressing, e.g. estimation, inference and operations with models, see e.g. [4–6,8,12,15].

This paper is structured as follows. A framework for models with COBS and some of their interesting results is provided in Section 2. Section 3 is dedicated to our main goal, which is to present a commutativity condition and other results enabling the obtention of BLUE. A real data application, considering an experiment with grapevines, is presented in Section 4 to illustrate the usefulness of the methodology. We conclude this work in Section 5, with some comments.

2. Models with commutative orthogonal block structure

To study COBS we resort to an approach based on their algebraic structure, since this leads to interesting results on the estimation of variance components and on the building up of models, see [10].

Let us consider a linear mixed model

$$Y = \sum_{i=0}^{w} X_i \boldsymbol{\beta}_i, \tag{1}$$

where β_0 is fixed and β_1, \ldots, β_w are random vectors with null mean vectors, variance-covariance matrices $\sigma_1^2 I_{c_1} \ldots \sigma_w^2 I_{c_w}$, where $c_i = rank(X_i)$, $i = 1, \ldots, w$, and null cross-covariance matrices.

The mean vector of Y is

$$\mu = X_0 \beta_0 \tag{2}$$

and the variance-covariance matrix is given by

$$V(\sigma^2) = \sum_{i=1}^{w} \sigma_i^2 M_i, \tag{3}$$

where $M_i = X_i X_i^T$, i = 1, ..., w.

The space spanned by the mean vector μ is $\Omega = R(X_0)$, so the orthogonal projection matrix (OPM), on Ω , is

$$T = X_0(X_0^T X_0)^+ X_0^T = X_0 X_0^+,$$

see e.g. [5], where+denotes the Moore-Penrose inverse.

When the matrices M_1, \ldots, M_w commute, they generate a commutative Jordan algebra of symmetric matrices, CJAS, A, this is, a linear space constituted by symmetric matrices that commute and containing the squares of its matrices [11]. The CJAS, A has a unique basis, its principal basis, Q, constituted by known pairwise orthogonal orthogonal projection matrices, POPM, Q_1, \ldots, Q_m , see [17]. Thus the matrices M_i , $i = 1, \ldots, w$, are linear

combinations of the matrices of the principal basis of the CJAS, which means that

$$M_i = \sum_{j=1}^m b_{i,j} \mathbf{Q}_j. \tag{4}$$

Considering $\gamma_j = \sum_{i=1}^w b_{i,j}\sigma_i^2$, j = 1, ..., m, the canonical variance components, the variance-covariance matrix of Y will take the form

$$V = \sum_{j=1}^{m} \gamma_j \mathbf{Q}_j. \tag{5}$$

When $\sum_{i=1}^{w} M_i$, belonging to θ , is invertible, θ is a complete CJAS and the matrices of its principal basis add up to the identity matrix, i.e.

$$\sum_{j=1}^{m} \mathbf{Q}_j = \mathbf{I}_n,\tag{6}$$

and model (1) is a model with OBS.

When dealing with OBS, inference usually involves orthogonal projections on the range spaces of the matrices Q_i , j = 1, ..., m, which is somewhat complex due to the combination of estimators obtained from different projections, see e.g. [4]. Imposing a commutativity condition on the OPM on the space spanned by the mean vector, T, and the POPM Q_i , $j = 1, \dots, m$, leads to a special class of OBS, those of models with COBS, see [10]. For this class of models we do not have the difficulty associated with orthogonal projections mentioned above, allowing, additionally, the least square estimators, for estimable vectors, to be UBLUE. According to the version of the Gauss-Markov theorem in [18], UBLUE are BLUE whatever the variance components.

3. Generalizing the commutativity condition

Assuming the rows of matrix X_0 to correspond to the sets of levels of the fixed effects factors, the mean values of the observations will be determined by those sets. Let us consider that there are \dot{n} sets of levels associated to r_1, \ldots, r_n , contiguous rows of X_0 . If the components of $\beta_0, \beta_{0,1}, \ldots, \beta_{0,n}$, are the corresponding mean values, we can reorder the observations to have the block diagonal matrix

$$X_0 = D(1_{r_1}, \dots, 1_{r_n}), \tag{7}$$

where 1_{r_l} , corresponds to the vector with all r_l components equal to $1, l = 1, ..., \dot{n}$. So, the orthogonal projection matrix on the space spanned by the mean vector, is given by

$$T = D\left(\frac{1}{r_1}J_{r_1}, \dots, \frac{1}{r_n}J_{r_n}\right) \tag{8}$$

where $J_{r_l} = 1_{r_l} 1_{r_l}^T$, $l = 1, ..., \dot{n}$.

The fundamental partition of Y will be constituted by the sub-vectors Y_1, \ldots, Y_n , corresponding to the n sets of the levels of the fixed effects factors, see [16]. Then the variance-covariance matrix can be defined by

$$V = \begin{bmatrix} V_{1,1} & \dots & V_{1,\hat{n}} \\ \vdots & & \vdots \\ V_{\hat{n},1} & \dots & V_{\hat{n},\hat{n}} \end{bmatrix}, \tag{9}$$

with $V_{l,l}$ the variance-covariance matrix of Y_l , $l=1,\ldots,\dot{n}$, and $V_{l,h}$ the cross-covariance matrix of Y_l and Y_h , $l\neq h$.

When T, the OPM on the space spanned by the mean vector μ , commutes with the POPM \mathbf{Q}_j , j = 1, ..., m, the OPM also commutes with the variance-covariance matrix of Y, V.

From (8) and (9) we have

$$TV = \begin{bmatrix} \frac{1}{r_1} J_{r_1} V_{1,1} & \dots & \frac{1}{r_1} J_{r_1} V_{1,\dot{n}} \\ \vdots & & \vdots \\ \frac{1}{r_{\dot{n}}} J_{r_{\dot{n}}} V_{\dot{n},1} & \dots & \frac{1}{r_{\dot{n}}} J_{r_{\dot{n}}} V_{\dot{n},\dot{n}} \end{bmatrix}$$
(10)

and

$$VT = \begin{bmatrix} V_{1,1} \frac{1}{r_1} J_{r_1} & \dots & V_{1,\hat{n}} \frac{1}{r_{\hat{n}}} J_{r_{\hat{n}}} \\ \vdots & & \vdots \\ V_{\hat{n},1} \frac{1}{r_1} J_{r_1} & \dots & V_{\hat{n},\hat{n}} \frac{1}{r_{\hat{n}}} J_{r_{\hat{n}}} \end{bmatrix}$$
(11)

So, the matrices *T* and *V* commute if and only if

$$\begin{cases}
\frac{1}{r_{1}}J_{r_{1}}V_{1,1} = V_{1,1}\frac{1}{r_{1}}J_{r_{1}} & \dots & \frac{1}{r_{1}}J_{r_{1}}V_{1,\dot{n}} = V_{1,\dot{n}}\frac{1}{r_{\dot{n}}}J_{r_{\dot{n}}} \\
\vdots & \vdots & \vdots & \ddots \\
\frac{1}{r_{\dot{n}}}J_{r_{\dot{n}}}V_{\dot{n},1} = V_{\dot{n},1}\frac{1}{r_{1}}J_{r_{1}} & \dots & \frac{1}{r_{\dot{n}}}J_{r_{\dot{n}}}V_{\dot{n},\dot{n}} = V_{\dot{n},\dot{n}}\frac{1}{r_{\dot{n}}}J_{r_{\dot{n}}}
\end{cases} (12)$$

These equalities imply that we must have

$$r_1 = \ldots = r_n = r$$

and equalities (12) may be condensed into

$$J_r V_{l,h} = V_{l,h} J_r, l, h = 1, \dots, \dot{n}.$$
 (13)

Now, given a matrix

$$U = \begin{bmatrix} u_{1,1} & \dots & u_{1,r} \\ \vdots & & \vdots \\ u_{r,1} & \dots & u_{r,r} \end{bmatrix}$$
 (14)

we have

$$J_{r}U = \begin{bmatrix} \sum_{l=1}^{r} u_{l,1} & \dots & \sum_{l=1}^{r} u_{l,r} \\ \vdots & & \vdots \\ \sum_{l=1}^{r} u_{l,1} & \dots & \sum_{l=1}^{r} u_{l,r} \end{bmatrix}$$
(15)

and

$$UJ_{r} = \begin{bmatrix} \sum_{h=1}^{r} u_{1,h} & \dots & \sum_{h=1}^{r} u_{1,h} \\ \vdots & & \vdots \\ \sum_{h=1}^{r} u_{r,h} & \dots & \sum_{h=1}^{r} u_{r,h} \end{bmatrix}.$$
 (16)

So, to have the equality

$$J_r U = U J_r \tag{17}$$

we must have

$$\sum_{l'=1}^{r} u_{l',h} = \sum_{h'=1}^{r} u_{l,h'} = \frac{\bar{u}}{r}, l, h = 1, \dots, r,$$

with $\bar{u} = \sum_{l'=1}^r \sum_{h'=1}^r u_{l',h'}$, which means that the sums of the elements in any row or column of matrix U are equal. Thus, matrix U is called a U-matrix, see [16].

Going back to the product of matrices V and T, we see that these matrices commute if and only if the sub-matrices $V_{l,h}$, l, h = 1, ..., m, are U-matrices. We thus have the following result.

Proposition 1: For the LSE of β_0 be UBLUE it is necessary and sufficient that $r_1 = \ldots =$ $r_n = r$ and the sub-matrices $V_{l,h}$, l, h = 1, ..., n be U-matrices.

Since we have

$$X_0 = D(1_r, \dots, 1_r) = I_m \otimes 1_r,$$
 (18)

where \otimes denotes the Kronecker matrices product, and taking $\dot{n} = m$ we also have

$$(X_0^T X_0)^{-1} = -\frac{1}{r} I_m,$$
 (19)

and so $(X_0^T X_0)^{-1} X_0^T = (1/r)D(1_r, \dots, 1_r)$. Thus, the components of

$$\widetilde{\beta}_{0} = (X_{0}^{T}X_{0})^{-1}X_{0}^{T}(Y_{1}^{T}...Y_{m}^{T})^{T}$$

will be the mean values $y_{0,1}, \ldots, y_{0,m}$ of the components of the sub-vectors Y_1, \ldots, Y_m .

We are thus led to replace $\boldsymbol{\beta}_0$ and $\widetilde{\boldsymbol{\beta}}_0$ by $\boldsymbol{\mu}_0 = (\boldsymbol{\mu}_{0,1}, \dots, \boldsymbol{\mu}_{0,m})$ and $\widetilde{\boldsymbol{\mu}}_0 = (\widetilde{\boldsymbol{\mu}}_{0,1}, \dots, \widetilde{\boldsymbol{\mu}}_{0,m})$, respectively, which enables us to consider other parametrizations, taking

$$\mu_0 = G\beta_0, \tag{20}$$

where G will have linearly independent column vectors. Then $\tilde{\mu}_0$ will be the matrix of sub-vectors means and, since

$$\boldsymbol{\beta}_0 = \boldsymbol{G}^+ \boldsymbol{\mu}_0 \tag{21}$$

we have the estimator

$$\widetilde{\boldsymbol{\beta}}_0 = \boldsymbol{G}^+ \tilde{\boldsymbol{\mu}}_0. \tag{22}$$

We also have the following proposition.

Proposition 2: The estimator $\widetilde{\beta}_0$ is UBLUE.

Proof: Let $\boldsymbol{\beta}_0^*$ be another unbiased estimator of $\boldsymbol{\beta}_0$. Then, for $\boldsymbol{c}^T\boldsymbol{\beta}_0$ we have the unbiased estimator $\boldsymbol{c}^T\boldsymbol{\beta}_0 = \boldsymbol{a}^T\tilde{\boldsymbol{\mu}}_0$ with $\boldsymbol{a}^T = \boldsymbol{c}^T\boldsymbol{G}^+$ and $\boldsymbol{c}^T\boldsymbol{\beta}_0^* = \boldsymbol{a}^T\boldsymbol{\mu}_0^*$, with $\boldsymbol{\mu}_0^* = \boldsymbol{G}\boldsymbol{\beta}_0^*$. Since $\boldsymbol{\mu}_0^*$ is an unbiased estimator of $\boldsymbol{\mu}_0$, and $\tilde{\boldsymbol{\mu}}_0$ is UBLUE for $\boldsymbol{\mu}_0$, we have $Var(\boldsymbol{c}^T\boldsymbol{\beta}_0^*) \leq Var(\boldsymbol{c}^T\boldsymbol{\beta}_0^*)$ whatever the variance components. Given that \boldsymbol{c} is arbitrary, $\tilde{\boldsymbol{\beta}}_0$ is BLUE. Since this holds for all variance components $\tilde{\boldsymbol{\beta}}_0$ is UBLUE.

Similarly, we may consider

$$\lambda = U\mu_0,\tag{23}$$

with the column vectors of U linearly independent. We now have the result.

Proposition 3: $\tilde{\lambda} = U\tilde{\mu}_0$ will be UBLUE for λ .

Proof: Since the column vectors of U are linearly independent we have $\mu_0 = U^+ \lambda$ and $\tilde{\mu}_0 = U^+ \tilde{\lambda}$. Given λ^* an unbiased estimator of λ , $\mu_0^* = U^+ \lambda^*$ will be an unbiased estimator of λ since its mean vector will be $U^+ U \mu_0 = \mu_0$. We also have $\lambda^* = U \mu_0^*$. Moreover, for $c^T \lambda$ we have the unbiased estimators $c^T \tilde{\lambda} = c^T U \tilde{\mu}_0 = (U^T c)^T \tilde{\mu}_0$ and $c^T \lambda^* = c^T U \mu_0^* = (U^T c)^T \mu_0^*$. Since $\tilde{\mu}_0$ is BLUE for μ_0 , we have $Var(c^T \tilde{\lambda}) \leq Var(c^T \lambda^*)$, whatever c, which shows that $\tilde{\lambda}$ is BLUE. Since this holds for all variance components $\tilde{\lambda}$ is UBLUE.

4. An application

Let's consider an experiment with 'Touriga Nacional' grapevine and two fixed effects factors:

- *Location* (in the experiment), with three levels;
- *Origin*, with two levels.

These two factors cross. Given the great number of clones, some ones were randomly chosen and considered as the levels of a random effects factor nested in the factor *Origin*.

LOCATION	ORIGIN 1			ORIGIN 2		
	Clone 1	Clone 2	Clone 3	Clone 1	Clone 2	Clone 3
1	3,00	1,00	1,10	1,75	1,10	1,05
	1,85	1,10	1,50	3,50	1,05	1,25
	0,75	1,00	1,80	2,50	0,50	2,00
	1,35	1,60	1,45	2,00	1,05	1,50
	1,45	1,50	1,25	0,65	1,25	2,10
2	1,80	1,60	0,85	2,00	1,20	1,00
	0,70	1,75	0,65	3,00	1,35	2,70
	2,50	0,50	0,55	2,55	1,20	2,15
	1,70	1,35	0,90	3,00	0,30	2,10
	0,40	1,10	0,09	2,65	2,50	2,70
3	1,05	0,75	0,90	1,60	1,05	1,60
	1,50	0,65	0,90	3,05	1,95	1,10
	1,15	0,90	0,55	0,25	2,00	2,05
	0,85	0,85	0,70	1,66	2,20	1,50
	1,15	1,05	0,35	2,65	2,35	3,00

Table 1. Production in Kg.

For each origin, three clones were randomly chosen. Lastly five grapevines were considered for each clone in each location. This experiment was analyzed, see [7,9], using its algebraic structure, namely using CJA. For completeness sake we now apply our approach.

We have $\dot{n} = 3 \times 2 = 6$ sub-vectors each with $r = 3 \times 5 = 15$ observations. These vectors are presented in Table 1.

With μ : the general mean; α_i : the effect of the i-th location, i=1,2,3; β_j : the effect of the j-th origin, j=1,2; $\gamma_{i,j}$: the interaction between the i-th location and the j-th origin, i=1,2,3, j=1,2; al,j: the random effect of the l-th clone of the j-th origin, l=1,2,3; j=1,2; we have, for the sub-vectors, the model equation

$$\mathbf{Y}_{i,j} = (\mu + \alpha_i + \beta_j + \gamma_{i,j})\mathbf{1}_{15} + \begin{bmatrix} a_{1,j} \\ a_{2,j} \\ a_{3,j} \end{bmatrix} \otimes \mathbf{1}_5 + \mathbf{e}_{i,j}; i = 1, 2, 3; j = 1, 2,$$
 (24)

where the $e_{i,j}$, i = 1, 2, 3, j = 1, 2, will be normal with null mean vector and variance-covariance matrix $\sigma_l^2 I_{15}$ independent from the vector \mathbf{a}_j , with components $(a_{1,j}, a_{2,j}, a_{3,j})$, j = 1, 2, which will be normal with null mean vector and covariance matrix $\sigma_a^2 I_3$. We can order these sub-vectors using the index l = 2(i - 1) + j; i = 1, 2, 3; j = 1, 2.

It is straightforward to obtain the covariance and cross-covariance matrices of the subvectors. We thus get

$$V_{1,1} = V_{2,2} = V_{3,3} = V_{4,4} = V_{5,5} = V_{6,6} = \sigma_a^2 I_3 \otimes J_5 + \sigma_l^2 I_{15}$$
 $V_{1,2} = V_{2,1} = V_{3,4} = V_{4,3} = V_{5,6} = V_{6,5} = 0_{15,15}$
 $V_{1,3} = V_{3,1} = V_{1,5} = V_{5,1} = V_{2,4} = V_{4,2} = \sigma_a^2 I_3 \otimes I_5$
 $V_{1,4} = V_{4,1} = V_{2,3} = V_{3,2} = V_{1,6} = V_{6,1} = 0_{15,15}$
 $V_{1,6} = V_{6,1} = V_{2,5} = V_{5,2} = V_{3,6} = V_{6,3} = 0_{15,15}$

It is easy to see that all these matrices are U-matrices. Thus, the LSE estimator of the vector μ_0 with components

$$\mu_{i,j} = \mu + \alpha_i + \beta_j + \gamma_{i,j}; i = 1, 2, 3; j = 1, 2$$
 (25)

will be UBLUE.

In this application we will focus in the LSE for β . The ANOVA analysis is standard. It is interesting to point out that, since

$$X_0 = D(1_r, \dots, 1_r) = I_m \otimes 1_r, \tag{26}$$

we have

$$(\mathbf{X_0}^T \mathbf{X_0})^{-1} \mathbf{X_0}^T = \frac{1}{r} D(1_r, \dots, 1_r) = \frac{1}{r} \mathbf{I}_m \otimes 1_r.$$
 (27)

Thus, the components of $\tilde{\beta}_0$ will be the means of the components of sub-vectors. We will represent those means by $\tilde{\mu}_{i,j}$, i=1,2,3; j=1,2. Taking

$$\begin{cases} \tilde{\mu}_{i,.} = \frac{1}{2}(\tilde{\mu}_{i,1} + \tilde{\mu}_{i,2}), i = 1, 2, 3\\ \tilde{\mu}_{.,j} = \frac{1}{3}(\tilde{\mu}_{1,j} + \tilde{\mu}_{2,j} + \tilde{\mu}_{3,j}), j = 1, 2\\ \tilde{\mu}_{...} = \frac{1}{6}\sum_{i=1}^{3}\sum_{j=1}^{2}\tilde{\mu}_{i,j} \end{cases}$$

we get the estimators

$$\begin{cases} \tilde{\alpha}_{i} = \tilde{\mu}_{i,.} - \tilde{\mu}_{.,.}, i = 1, 2, 3\\ \tilde{\beta}_{j} = \tilde{\mu}_{.,j} - \tilde{\mu}_{.,.}, j = 1, 2\\ \tilde{\gamma}_{i,j} = \tilde{\mu}_{i,j} - \tilde{\mu}_{i,.} - \tilde{\mu}_{.,j} + \tilde{\mu}_{.,.}, i = 1, 2, 3; j = 1, 2 \end{cases}$$

According to Proposition 1 these estimators will be UBLUE.

Besides this, using software R, we carried out a standard ANOVA whose main results are presented in Table 2.

From the results presented in Table 2, we conclude that interaction between the fixed effects factors (Location and Origin) and Location are significant.

5. Final comments

The use of linear mixed models is suitable for correlated data due to, for example, repeated measurements. From Nelder's work emerged a particular class of linear mixed models, named OBS, that took a central role in the theory of randomized block designs, giving rise to several lines of research. As a relevant step towards the adequacy of the estimators came a special class of OBS, called COBS, which allows the estimation of relevant parameters to be optimized. COBS are based on commutativity between T, the OPM on the space spanned by the mean vector, and the POPM Q_j , $j=1,\ldots,m$. The commutativity condition we presented is easy to verify and guaranties UBLUE estimators, obtained through least squares, for the coefficients vector and estimable vectors. Thus, we consider that our aims were attained.



Table 2. Model summary and ANOVA table.

	•								
Linear mixed m lmerModLmerTes Formula: Grape	st] evines \sim I	_ Location * (Origin + (1			[
REML criterior	n at conve	rgence: 179	. 5						
Scaled residua	als:								
Min		1Q	Median		3 Q	Max			
-3.2873	-0.53	57	-0.0656	0	.5693	2.5275			
Random effects	S:								
Groups	Name			Variance		Std.Dev.			
Origin:Clone		(Interce	ept)	0.02634	0.1623				
Clone	(Interce		ept)	0.05287	0.2299				
Residual			-	0.37638	0.6135				
Number of obs:	Number of obs: 90, groups: Origin:Clone, 6; Clone, 3								
Fixed effects:	:								
	Esti	mate Std.	Error	df t	value	Pr(> t)			
(Intercept)	1.9449		0.5952	30.7182	3.268	0.00267 **			
Location	-0.7187		0.2505	81.9992-2.869		0.00523 **			
Origin	-0.2238		0.3670	25.5218-0.610		0.54737			
Location:Origi	in 0.43	87	0.1584	81.9992	2.769	0.00695 **			
 Signif. codes:	: 0 `***′ ().001 `**′ (0.01 *′ 0.	05 `.′ 0.1	` ` 1				
Correlation of	Fixed Eff	ects:							
		(Intr)		Locatn		Origin			
Location		-0.842				- 3			
Origin		-0.925		0.819					
Locatn:Orgn		0.798		-0.949		-0.863			
	Sum Sq	Mean Sq	NumDF	DenDF	F value	Pr(> F)			
Location	3.0988907	3.0988907	1	81.99925	8.2333400	0.005229186			
Origin	0.1399722	0.1399722	1	25.52179	0.3718876	0.547368822			
Location:Origin	2.8864267	2.8864267	1	81.99925	7.6688514	0.006945885			

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No potential conflict of interest was reported by the author(s).

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