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STRICTLY ASSOCIATED MODELS, PRIME BASIS FACTORIALS: AN APPLICATION

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Abstract

Mixed models will be considered using the Commutative Jordan Algebra of Symmetric matrices approach. Prime basis factorial models will now be considered in the framework provided by Commutative Jordan Algebra of Symmetric matrices. This will enable to obtain fractional replicates when the number of levels is neither a prime or a power of a prime. We present an application to the effect of lidocaine, at an enzymatic level, on the heart muscle of beagle dogs

Keywords: COBS, strictly associated models, prime basis factorials, inference.

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1. Introduction

We start by using Commutative Jordan Algebras of Symmetric matrices (CJAS) to study the algebraic structure of orthogonal models. The CJAS were introduced by Jordan *et al.* (1934), see [4], in order to provide an algebraic formulation for quantum mechanics, only later on they were rediscovered by Seely (1970a) [7], (1970b) [8], (1971) [9], Seely & Zyskind (1971) [10] and used in statistics. These algebras are vector spaces constituted by symmetric matrices that commute and containing the squares of their matrices.

An orthogonal model

$$\mathbf{y} = \sum_{i=1}^{w} \mathbf{X}_i \boldsymbol{\beta}_i$$

is associated to an CJAS $\mathscr{A}$, if the family $\mathscr{T} = \{\mathbf{M}_1, \ldots, \mathbf{M}_w\}$, with $\mathbf{M}_i = \mathbf{X}_i \mathbf{X}_i^\top$, $i = 1, \ldots, w$, is a basis for $\mathscr{A}$ with $\mathscr{V} = \{\mathbf{Q}_1, \ldots, \mathbf{Q}_w\}$ the principal basis of $\mathscr{A}$ we will have

$$\mathbf{M}_i = \sum_{j=1}^{w} b_{i,j} \mathbf{Q}_j,$$

the transition matrix $\mathbf{B} = [b_{i,j}]$ being regular. In our study we will derive conditions on the algebraic structure of orthogonal models, normally on their transition matrices, to enable the proper treatment of mixed models. Moreover we can always write $\mathbf{Q}_j = \mathbf{A}_j^\top \mathbf{A}_j$ with $\mathbf{A}_j$ such that $\mathbf{A}_j \mathbf{A}_j^\top = \mathbf{I}_{g_j}$, $j = 1, \ldots, w$, it being highly convenient that the model is separated that is that

$$\mathbf{A}_j \mathbf{X}_i \boldsymbol{\beta}_i = \mathbf{0}_{g_j} \qquad j \neq i.$$

In the last part of our study we will consider prime basis factorials models in the framework provided by CJAS. This will enable to obtain fractional replicates when the number of levels is neither a prime or a power of a prime. Lastly we consider an application on the lidocaine at an enzymatic level, on the heart muscle of beagle dogs.

2. Algebraic Structure

Let

$$\mathbf{P} = \left[\mathbf{A}_1^\top, \ldots, \mathbf{A}_w^\top\right]^\top \tag{1}$$

be an orthogonal matrix associated to a commutative Jordan algebra $\mathscr{A}$, constituted by $m \times m$ matrices.

With $\mathbf{K}_s$ a matrix, obtained by removing the first line, $\frac{1}{\sqrt{s}}\mathbf{1}_s^\top$, of a $s \times s$ orthogonal matrix,

$$\overline{\mathbf{P}} = \left[\mathbf{A}_1^\top \otimes \frac{1}{\sqrt{s}} 1_s, \ldots, \mathbf{A}_w^\top \otimes \frac{1}{\sqrt{s}} 1_s, \mathbf{A}^{\perp\top}\right]^\top \tag{2}$$

where $\otimes$ represents the usual kronecker matrices product and $\mathbf{A}^{\perp} = \mathbf{I}_m \otimes \mathbf{K}_s$ will be an orthogonal matrix associated to $\mathscr{A} \star \mathscr{A}(s)$, where $\star$ represents the restricted kronecker product, see *e.g.* Fonseca *et al.* (2006). We also have

$$\overline{\mathbf{J}}_s = \mathbf{I}_s - \frac{1}{s}\mathbf{J}_s = \mathbf{K}_s^{\top}\mathbf{K}_s. \tag{3}$$

A model with $m = n \times s$ observations, is strictly associated to $\mathscr{A}$, if it can be written as

$$\mathbf{y} = \sum_{i=1}^{w} \left(\mathbf{A}_j^{\top} \otimes \frac{1}{\sqrt{s}} 1_s \right) \widetilde{\boldsymbol{\eta}}_j + \boldsymbol{\varepsilon}, \tag{4}$$

where $\widetilde{\boldsymbol{\eta}}_j \sim N\left(\boldsymbol{\eta}_j, \gamma_j \mathbf{I}_{g_j}\right)$, $j = 1, \ldots, w$, and $\boldsymbol{\varepsilon} \sim N\left(\mathbf{0}, \mathbf{Q}^{\perp}\right)$, with $\mathbf{Q}^{\perp} = \mathbf{A}^{\perp^{\top}}\mathbf{A}^{\perp}$, and these vectors are independent. This model will have m fixed effects terms, if

$$\begin{cases} \boldsymbol{\eta}_j = \mathbf{0}\,, & j = m+1, \ldots, w, \\ \boldsymbol{\gamma}_j = \boldsymbol{\sigma}^2, & j = 1, \ldots, m. \end{cases} \tag{5}$$

The models we are dealing with will have fixed effects, random effects or mixed effects, according to

$$\begin{cases} m = w & \text{fixed effects} & \gamma_j = \sigma^2, & j = 1, \ldots, w, \\ 1 < m < w & \text{mixed effects} & \gamma_j = \sigma^2, & j = 1, \ldots, m, \\ & & \boldsymbol{\eta}_j = \mathbf{0}, & j = m+1, \ldots, w, \\ 1 = m & \text{random effects} & \boldsymbol{\eta}_j = \mathbf{0}, & j = 2, \ldots, w. \end{cases}$$

3. Inference

Let's put $g_j = \operatorname{rank}(\mathbf{Q}_j) = \operatorname{rank}(\mathbf{A}_j)$, $j = 1, \ldots, w$, and $g = \operatorname{rank}(\mathbf{Q}^{\perp}) = \dot{n}(s-1)$, with $\dot{n}$ the number of treatments. Thus we will have

$$
(6)\qquad \begin{cases} \mathbf{V}^{-1} = \displaystyle\sum_{j=1}^{w} \gamma_j^{-1} \left(\mathbf{Q}_j \otimes \frac{1}{s} \mathbf{J}_s \right) + \frac{1}{\sigma^2} \mathbf{Q}^{\perp}, \\ \det(\mathbf{V}) = \displaystyle\prod_{j=1}^{w} \gamma_j^{g_j} (\sigma^2)^g \end{cases}
$$

as well as

$$
(7)\qquad \begin{aligned} (\mathbf{y} - \boldsymbol{\mu})^{\top} \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu}) &= \sum_{j=1}^{w} \frac{1}{\gamma_j} \|\widetilde{\boldsymbol{\eta}}_j - \boldsymbol{\eta}_j\|^2 + \frac{S}{\sigma^2} \\ &= \sum_{j=1}^{m} \frac{1}{\gamma_j} \|\widetilde{\boldsymbol{\eta}}_j - \boldsymbol{\eta}_j\|^2 + \sum_{j=m+1}^{w} \frac{S_j}{\gamma_j} + \frac{S}{\sigma^2} \end{aligned}
$$

with $S_j = \|\widetilde{\boldsymbol{\eta}}_j\|^2$, $j = 1, \ldots, w$ and $S = \|\boldsymbol{\varepsilon}^{\perp}\|^2 = \|\mathbf{Q}^{\perp}\mathbf{y}\|^2$. Then we can write the probability density function as

$$
(8)\qquad n(\mathbf{y}) = \frac{e^{-\frac{1}{2}\left(\sum_{j=1}^{m} \frac{1}{\sigma^2} \|\widetilde{\boldsymbol{\eta}}_j - \boldsymbol{\eta}_j\|^2 + \sum_{j=m+1}^{w} \frac{S_j}{\gamma_j} + \frac{S}{\sigma^2} \right)}}{(2\pi)^{\frac{n}{2}} \displaystyle\prod_{j=1}^{w} \gamma_j^{\frac{g_j}{2}} (\sigma^2)^g}
$$

so the $\widetilde{\boldsymbol{\eta}}_j$, $j = 1, \ldots, m$, the S_j, $j = m+1, \ldots, w$, and S constitute a sufficient and complete statistic, since the normal density belongs to the exponential family and the parametric contains the product of non degenerated intervals, see Lehman (1986, pag. 132) [5]. Moreover $\widetilde{\boldsymbol{\eta}}_j \sim \mathcal{N}\left(\boldsymbol{\eta}_j, \gamma_j \mathbf{I}_{g_j}\right)$, $j = 1, \ldots, w$, $S_j \sim \gamma_j \chi^2_{g_j}$, $j = m+1, \ldots, w$, and $S \sim \sigma^2 \chi^2_g$, so we have UMVUE for the estimable vectors and variance components.

4. Prime Basis Factorials

With p a prime number, p^N will be a model in which N factors with p levels cross. We now derive commutative Jordan algebras associated to such models.

The factor numbers may be numbered from 0 to $p-1$. Thus the p^N treatments may be represented by vectors $\underline{x}$ with components $x_j = 0, \ldots, p-1$, $j = 1, \ldots, N$. Let $\underline{x}_j$ be the vector with index

$$k(\underline{x}_j) = 1 + \sum_{j=1}^{N} p^{j-1} x_j \tag{9}$$

equal to j.

In the analysis of these models the functions

$$f(\underline{x}|\underline{a}) = \left(\sum_{j=1}^{N} a_j x_j \right)_{(p)}, \tag{10}$$

where $a_j = 0, \ldots, p-1$, $j = 1, \ldots, N$, play a central part, see for instance Jesus *et al.* (2009) [2]. The values of these functions are obtained using the module p arithmetic. To avoid redundancies only the functions where the first non null coefficient are considered. Let $\mathscr{L}$ be the set of such functions.

With $\mathbf{W}(f)$ the $p \times p^N$ matrix with elements

$$w_{i,j}(f) = \begin{cases} w_{i,j}(f) = 0, & f(\underline{x}_j) \neq i-1, \\ \\ w_{i,j}(f) = 1, & f(\underline{x}_j) = i-1, \end{cases} \tag{11}$$

the matrix

$$\mathbf{P} = \begin{bmatrix} \frac{1}{\sqrt{p^N}} \mathbf{1}_{p^N}^\top \\ \\ \mathbf{A}(f); f \in \mathscr{L} \end{bmatrix}, \tag{12}$$

where $\mathbf{A}(f) = \mathbf{K}_p \mathbf{W}(f)$, is orthogonal, see e.g., Jesus *et al.* (2009a) [2], Jesus *et al.* (2009b) [3]. This will be an orthogonal matrix associated to the CJAS $\mathscr{A}(p^N)$ with principal basis $\left\{ \frac{1}{p^N}\mathbf{J}, \mathbf{Q}(f), f \in \mathscr{L} \right\}$, where $\mathbf{Q}(f) = (\mathbf{A}(f))^\top \mathbf{A}(f)$. The model

$$\mathbf{y} = \frac{1}{p^{N/2}} \mathbf{1}_{p^N} \otimes \mathbf{1}_r \mu + \sum_{f \in \mathscr{L}} \left((\mathbf{A}(f))^\top \boldsymbol{\beta}(f) \right) \otimes \mathbf{1}_r + \boldsymbol{\varepsilon} \tag{13}$$

will be associated to the CJAS $\mathscr{A}(p^N) \star \mathscr{A}(r)$. It is interesting to point out that, in this case, basis $\mathscr{T}$ and $\mathscr{V}$ of $\mathscr{A}(p^N)$ are identical. Thus the model is triangular and, in the mixed case, segregated.

4.1. Random effects models

The random vectors in the canonical form are now the

$$\begin{cases} \boldsymbol{\beta}(\ell) \sim \mathcal{N}\left(\mathbf{0}, \gamma(\ell)\mathbf{l}_{p-1}\right), \\ \varepsilon \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}_n\right) \end{cases}$$

with $\boldsymbol{\beta}_\ell$ independent from $\boldsymbol{\varepsilon}$, as well as

$$\begin{cases} S_\ell = \|\mathbf{A}(\ell)\mathbf{y}\|^2 \sim \left(\gamma(\ell) + \sigma^2\right)\chi^2_{p-1}, \\ S = \left\|\mathbf{A}^\perp\mathbf{y}\right\|^2 \sim \sigma^2\chi^2_g, \end{cases}$$

where S_ℓ is independent from S, which give us the UMVUE,

$$\begin{cases} \widetilde{\sigma}^2 = \dfrac{S}{g}, \\ \widetilde{\gamma}(l) = \dfrac{S_l}{p-1} - \dfrac{S}{g}, \end{cases} \tag{14}$$

since

$$\begin{cases} \mathbb{E}\left(\dfrac{S_\ell}{p-1}\right) = \gamma(\ell) + \sigma^2, \\ \mathbb{E}\left(\dfrac{S_\ell}{p-1} - \dfrac{S}{g}\right) = \gamma(\ell). \end{cases} \tag{15}$$

Besides this

$$\mathscr{F}(\ell) = \frac{g}{p-1}\frac{S_\ell}{S}$$

will be the product by $\theta(\ell) = \dfrac{\sigma^2 + \gamma(\ell)}{\sigma^2}$, of a central F variable with $p-1$ and g degrees of freedom. Thus $\mathscr{F}(\ell)$ will be used to test

$$\begin{cases} H_0(\ell) : \gamma(\ell) = 0 \\ \text{or} \\ H_0(\ell) : \theta(\ell) = 1 \end{cases}$$

against

$$\begin{cases} H_1(\ell) : \gamma(\ell) > 0 \\ \text{or} \\ H_1(\ell) : \theta(\ell) > 1. \end{cases}$$

Since

$$\mathscr{F}(\ell) \sim F\left(\frac{z}{\theta(\ell)} \,|p-1, g\right)$$

this test is strictly unbiased.

4.2. Fixed and random models

In this case $\mathscr{L}^\circ = \mathscr{L}_f \cup \mathscr{L}_r$, with $\boldsymbol{\beta}(\ell)$ fixed when $\ell \in \mathscr{L}_f$ and $\boldsymbol{\beta}(\ell) \sim \mathcal{N}\left(\mathbf{0}, \sigma^2(\ell)\mathbf{I}_{p-1}\right)$ when $\ell \in \mathscr{L}_a$. For $\ell \in \mathscr{L}_f$ or $\ell \in \mathscr{L}_r$ we can use the previous results.

4.3. Replicates

We now have r "copies" of the base model, that is strictly associated to a CJAS. We assume the "copies" to correspond to the levels of a fixed effects factor that does not interact with the factors in the base model. In the first step in the analysis we take the n° treatments in the base models as levels of a factor. We then would have two factors, which do not interact, with n° and r level factor. In the second step if the model is strictly associated to a CJAS with principal basis $\{\mathbf{Q}_1, \ldots, \mathbf{Q}_w\}$,having

$$\begin{cases} \mathbf{Q}_1 = \dfrac{1}{n^\circ}\mathbf{J}_{n^\circ}, \\ \\ \displaystyle\sum_{j=2}^{w} \mathbf{Q}_j = \overline{\mathbf{J}}_{n^\circ}. \end{cases} \tag{16}$$

The model with replicates will be strictly associated to $\mathscr{A}^{\circ}$, if

$$\mathbf{Q}_j = \mathbf{A}_j^{\top}\mathbf{A}_j, \qquad j = 1, \ldots, w, \tag{17}$$

we will have

$$\begin{cases} \frac{1}{n^{\circ}}\mathbf{J}_{n^{\circ}} \otimes \frac{1}{r}\mathbf{J}_r = \left(\frac{1}{\sqrt{n^{\circ}}}\mathbf{1}_{n^{\circ}} \otimes \frac{1}{\sqrt{r}}\mathbf{1}_r\right)\left(\frac{1}{\sqrt{n^{\circ}}}\mathbf{1}_{n^{\circ}}^{\top} \otimes \frac{1}{\sqrt{r}}\mathbf{1}_r^{\top}\right), \\ \frac{1}{n^{\circ}}\mathbf{J}_{n^{\circ}} \otimes \overline{\mathbf{J}}_r = \left(\frac{1}{\sqrt{n^{\circ}}}\mathbf{1}_{n^{\circ}} \otimes \mathbf{K}_r^{\top}\right)\left(\frac{1}{\sqrt{n^{\circ}}}\mathbf{1}_{n^{\circ}}^{\top} \otimes \mathbf{K}_r\right), \\ \mathbf{Q}_j \otimes \frac{1}{r}\mathbf{J}_r = \left(\mathbf{A}_j^{\top} \otimes \frac{1}{\sqrt{r}}\mathbf{1}_r\right)\left(\mathbf{A}_j \otimes \frac{1}{\sqrt{r}}\mathbf{1}_r^{\top}\right), \quad j = 2, \ldots, w, \\ \overline{\mathbf{J}}_{n^{\circ}} \otimes \overline{\mathbf{J}}_r = \left(\mathbf{T}_{n^{\circ}}^{\top} \otimes \mathbf{T}_r^{\top}\right)\left(\mathbf{K}_{n^{\circ}} \otimes \mathbf{K}_r\right) \end{cases} \tag{18}$$

and we can now apply a similar treatment to the one presented before. The first of these matrices will be associated to the general mean value, the second one to the replicates, the next one to the effects and interactions of the factors in the base model and the last one to the error.

5. An application

The application that we are about to consider, is a 3^3 design, for the study of the effect of lidocaine, at an enzymatic level, on the heart muscle of beagle dogs, see Montgomery (2005) [6]. Three different brands of lidocaine were used as well as three different doses and three dogs. The first two factors had fixed effects and the last one random effects. Two replicates were carried out. We present the data in Table 1.

On the next table we can see the F tests and their $p - values$. The leading factor is clearly dose. Moreover there is some interaction between brand and dose. To complete the analysis of the factor dose we obtained it's linear and quadratic effects and tested them. The F tests were 714,06 and 2,36 with *p-value* ≈ 0 and $0,13656$. So only the linear effect was significant.

Table 1. Enzyme levels.

		Replica 1			Replica 2		
		Dog			Dog		
Brand	Dosage	1	2	3	1	2	3
1	1	86	84	85	84	85	86
	2	94	99	98	95	97	90
	3	101	106	98	105	104	103
2	1	85	84	86	80	82	84
	2	95	98	97	93	99	95
	3	108	114	109	110	102	100
3	1	84	83	81	83	80	79
	2	95	97	93	92	96	93
	3	105	100	106	102	111	108

Table 2. F Tests and $p - values$.

Reduced Application	Sum of Squares	F tests	$p - value$
x_1	31,00	2,59	0,0936
x_2	4260,80	357,03	$\simeq 0$
$x_1 + x_2$	51,42	4,31	0,0242
$x_1 + 2x_2$	18,14	1,52	0,2375
x_3	28,00	2,35	0,1157
$x_1 + x_3$	0,83	0,07	0,9327
$x_1 + 2x_3$	2,50	0,21	0,8124
$x_2 + x_3$	25,50	2,14	0,1383
$x_2 + 2x_3$	11,39	0,95	0,3982
$x_1 + x_2 + x_3$	25,25	2,21	0,1408
$x_1 + x_2 + 2x_3$	4,42	0,37	0,6943
$x_1 + 2x_2 + x_3$	4,03	0,34	0,7166
$x_1 + 2x_2 + 2x_3$	27,08	2,27	0,1235

6. Final remarks

The results obtained in this application are in line with the ones obtained using the classical approach, but the methodology presented here allows the study of a larger number of interactions simultaneously. Also, using COBS allows us to consider a third factor (the dogs), making this a more realistic model, being this way more advantageous the use of the technique presented here.

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