ALGEBRAIC STRUCTURE OF STEP NESTING DESIGNS

CÉLIA FERNANDES, PAULO RAMOS
Área Científica de Matemática, Instituto Superior de Engenharia de Lisboa
Rua Conselheiro Emídio Navarro, 01 1959–007 Lisboa, Portugal
e-mail: cfernandes@deetc.isel.ipl.pt
e-mail: pramos@deetc.isel.ipl.pt

AND

JOÃO TIAGO MEXIA
Departamento de Matemática
Faculdade de Ciências e Tecnologia Universidade Nova de Lisboa
Monte de Caparica 2829–516 Caparica, Portugal
e-mail: jtm@fct.unl.pt

Abstract

Step nesting designs may be very useful since they require fewer observations than the usual balanced nesting models. The number of treatments in balanced nesting design is the product of the number of levels in each factor. This number may be too large. As an alternative, in step nesting designs the number of treatments is the sum of the factor levels. Thus these models lead to a great economy and it is easy to carry out inference. To study the algebraic structure of step nesting designs we introduce the cartesian product of commutative Jordan algebras.

Key Words: commutative Jordan algebras, cartesian product of commutative Jordan algebras, step nesting, variance components, UMVUE.

1. Introduction

In the step nesting designs with \( u \) factors we have \( u \) steps, (see Cox et al., 2003). Each step corresponds to a one factor model. In the model corresponding to \( j^{th} \) step the first \( j - 1 \) factors have an unique level, then there are \( a(j) \) levels for the \( j^{th} \) factor which nest a single level of the following factor. If we have \( a(1), \ldots, a(u) \) “active” levels for the \( u \) factors that nest, in balanced nesting we have \( \prod_{i=1}^{u} a(i) \) combinations of levels and in step nesting we have \( \sum_{i=1}^{u} a(i) \) combinations.

We point out that the examples presented in Figures 1 and 2, correspond to designs with the same number of levels in each factor. In both case we consider the first factor with three levels, the second with four levels, the third factor with two levels and the fourth factor with five levels. It is easy to see that the number of treatments in a balanced nesting design is \( 3 \times 4 \times 2 \times 5 = 120 \). In step nesting designs we will have \( 3 + 4 + 2 + 5 = 14 \) treatments.

Figure 1. Designs with balanced nesting.

Figure 2. Designs with step nesting.
Algebraic structure of step nesting designs

The proposal in step nesting designs is to use $a_1$ levels for the first factor, combined with a single level of all other factors; then a new single level for the first factor, combined with $a_2$ new levels of the second factor, combined with a single level of all other factors; and so on.

Let $u$ be the number of factors with $a_1, \ldots, a_u$ “active” levels. The last factor may correspond to replicates.

In the $j^{th}$ factor we will have $c(j) = (u - j) + \sum_{k=1}^{j} a_k$ levels. For the design in the Figure 2 we have $c(1) = 6$, $c(2) = 9$, $c(3) = 10$ and $c(4) = 14$.

To study step nesting models we will use the cartesian product of commutative Jordan algebras. In the next section we present results on these algebras and introduce that operation. Thus we consider the algebraic structure of step nesting models and show how to carry out inference.

2. Commutative Jordan algebras

Commutative Jordan algebras (CJA) are linear spaces constituted by symmetric matrices that commute and contain the squares of their matrices. These structures were introduced by Jordan et al. (1934) in a reformulation of Quantum Mechanics. Later, they were rediscovered by Seely (1970a,b, 1971, 1972, 1977; Seely & Zyskind (1971), that used these algebras in Linear Statistical Inference, and later used by Zmyślony (1978), Drygas & Zmyślony (1992), Vanaleuween et al. (1998, 1999) and Malley (2004). Later, see eg, Michalski et al. (1996, 1999), they were used to construct hypothesis tests. Seely (1970a,b) named them as Quadratic Vector Spaces, which is also done by Rao & Rao (1998), but for priority sake we name them as Commutative Jordan Algebras. Some care must be observed here since Malley (2004) points out that there are linear spaces constituted by matrices, closed for the Jordan matrix product

\begin{equation}
A \triangledown B = \frac{1}{2}(AB + BA)
\end{equation}

and containing the squares of their matrices that, even when their matrices commute, are isomorphic to no CJA constituted by symmetric matrices. We thus will consider CJA constituted by symmetric matrices.
Any commutative Jordan algebra \( \mathcal{A} \) has one and only one basis, the principal basis \( \text{pb}(\mathcal{A}) \), constituted by pairwise orthogonal orthogonal projection matrices, see Seely (1971).

If the sum of the matrices in \( \text{pb}(\mathcal{A}) \) is the identity matrix, \( \mathcal{A} \) will be complete.

Since the matrices in \( \text{pb}(\mathcal{A}) \) are idempotent and pairwise orthogonal, any projection matrix belonging to \( \mathcal{A} \) is idempotent, so it will be the sum of all or part of the matrices in \( \text{pb}(\mathcal{A}) \). The rank of an orthogonal projection matrix will be the sum of the ranks of those matrices in \( \text{pb}(\mathcal{A}) \) which add to that matrix. Thus a orthogonal projection matrix with rank 1 will belong to \( \text{pb}(\mathcal{A}) \) whenever it belong to \( \mathcal{A} \). With \( \mathbf{1}^n \) the vector with \( n \) components equal to 1 and \( \mathbf{J}_n = \mathbf{1}^n(\mathbf{1}^n)' \), \( \frac{1}{n}\mathbf{J}_n \) will be a orthogonal projection matrix with rank 1 so that it belongs to \( \text{pb}(\mathcal{A}) \) whenever it belongs to \( \mathcal{A} \).

A commutative Jordan algebra of \( n \times n \) matrices that contains \( \frac{1}{n}\mathbf{J}_n \) will be regular.

The commutative Jordan algebra with principal basis \( \{ \frac{1}{r}\mathbf{J}_r; \mathbf{K}_r \} \), with \( \mathbf{K}_r = \mathbf{I}_r - \frac{1}{r}\mathbf{J}_r \), is a regular complete commutative Jordan algebra with dimension two. We have \( \mathbf{K}_r = (\mathbf{T}_r)'\mathbf{T}_r \) with \( \mathbf{T}_r \) the matrix obtained deleting the first row equal to \( \frac{1}{\sqrt{r}}(\mathbf{1}^r)' \) from an \( r \times r \) orthogonal matrix.

If \( Q = \text{pb}(\mathcal{A}) \) is constituted by matrices \( \mathbf{Q}_1, \ldots, \mathbf{Q}_k \) and the row vectors of \( \mathbf{A}_j \) constitute an orthogonal basis for the range space \( \text{R}(\mathbf{Q}_j) \) of \( \mathbf{Q}_j \), \( j = 1, \ldots, k \), we put \( \text{pb}(\mathcal{A})^2 = \{ \mathbf{A}_1, \ldots, \mathbf{A}_k \} \). We then have

\[
\begin{align*}
\mathbf{A}_j\mathbf{A}_j' &= \mathbf{I}_{g_j}, \quad j = 1, \ldots, k \\
\mathbf{A}_j\mathbf{A}_j' &= \mathbf{Q}_j, \quad j = 1, \ldots, k
\end{align*}
\]

(2.2)

with \( g_j = \text{rank}(\mathbf{Q}_j), \quad j = 1, \ldots, k \). Moreover since the \( \mathbf{Q}_1, \ldots, \mathbf{Q}_k \) are pairwise orthogonal we will have

\[
\mathbf{A}_j\mathbf{A}_{j'} = \mathbf{0}_{g_j \times g_{j'}}, \quad j \neq j'
\]

(2.3)

with \( \mathbf{0}_{r \times s} \) the \( r \times s \) null matrix.
Given $M$ a regular matrix belonging to $\mathcal{A}$, we have

\begin{equation}
M = \sum_{j=1}^{k} m_j Q_j
\end{equation}

with $Q_1, \ldots, Q_k$ the matrices in the principal basis of $\mathcal{A}$. Since the $Q_1, \ldots, Q_k$ are pairwise orthogonal and idempotent we will have

\begin{equation}
M^{-1} = \sum_{j=1}^{k} m_j^{-1} Q_j.
\end{equation}

Moreover, if $Q_j = A'_j A_j$, $j = 1, \ldots, k$, we will have

\begin{equation}
M = \sum_{j=1}^{k} m_j A'_j A_j
\end{equation}

so the row vectors of $A_j$ will be eigenvectors of $M$ associated to the eigenvalues $m_j$ with multiplicity $g_j = \text{rank}(A_j) = \text{rank}(Q_j)$, $j = 1, \ldots, k$, and so

\begin{equation}
\det(M) = \prod_{j=1}^{k} m_j^{g_j}.
\end{equation}

**Definition 1.** Let $D(B_1, \ldots, B_u)$ be the block-wise diagonal matrix with principal blocks $B_1, \ldots, B_u$. Given the commutative Jordan algebras, $\mathcal{A}_1, \ldots, \mathcal{A}_u$, their cartesian product will be the set of the $D(M_1, \ldots, M_u)$ with $M_h \in \mathcal{A}_h$, $h = 1, \ldots, u$. We will represent by $\times_{h=1}^{u} \mathcal{A}_h$ this cartesian product of commutative Jordan algebras.

Now we establish

**Proposition 1.** Let $\mathcal{A}_h$ be commutative Jordan algebra constituted by $a_h \times a_h$ matrices with principal basis $Q_h = \{Q_{h,1}, \ldots, Q_{h,v_h}\}$, then the principal basis of $\times_{h=1}^{u} \mathcal{A}_h$ will be $\bigcup_{h=1}^{u} Q_{a,h}$ with $Q_{a,h}$ the family of the $D(B_1, \ldots, B_u)$ with $B_{h'} = 0_{a_{h'} \times a_{h'}}$, if $h' \neq h$, and $B_h \in Q_h$, $h = 1, \ldots, u$. 

Proof. Clearly \( \bigcup_{h=1}^{u} Q_{a,h} \) is a family of pairwise orthogonal projection matrices contained in \( \times_{h=1}^{u} \mathcal{A}_h \). Moreover \( \bigcup_{h=1}^{u} Q_{a,h} \) contains \( \sum_{h=1}^{u} d_h \) matrices with \( d_h = \dim (\mathcal{A}_h) \), \( h = 1, \ldots, u \).

To complete the proof we have only to point out that whatever matrix in \( \times_{h=1}^{u} \mathcal{A}_h \) can be written in one and only one way as a linear combination of the matrices in \( \bigcup_{h=1}^{u} Q_{a,h} \).

\[ \blacksquare \]

3. Step nesting designs

3.1. Model

For these designs we have the random effects model

\[
y = \sum_{h=0}^{u} X(h) \beta(h),
\]

with, the block-wise diagonal matrices

\[
\begin{align*}
X(0) &= D(1^{a(1)}, \ldots, 1^{a(u)}) \\
X(h) &= D(I_{a(h)}, 1^{a(h+1)}, \ldots, 1^{a(u)}), \ h = 1, \ldots, u - 1 \\
X(u) &= D(I_{a(1)}, \ldots, I_{a(u)})
\end{align*}
\]

where \( 1^s \) is the vector with \( s \) components equal to 1 and \( I_s \) is the \( s \times s \) identity matrix.

We assume that \( \beta(0) = 1^u \mu \) with \( \mu \) the general mean value, and that the \( \beta(h) \), \( h = 1, \ldots, u \), are normal, independent with null mean vectors and variance-covariance matrices \( \sigma^2(h) I_{c(h)} \), \( h = 1, \ldots, u \), putting

\[
\beta(h) \sim \mathcal{N}(0^{c(h)}, \sigma^2(h) I_{c(h)}), \ h = 1, \ldots, u.
\]
Then \( y \sim \mathcal{N}(\mu, V) \), with

\[
\begin{align*}
\mu &= \mathbf{1}^n \mu \\
V &= \sum_{h=1}^{u} \sigma^2(h) M(h)
\end{align*}
\]

(3.11)

where \( M(h) = \mathbf{X}(h) [\mathbf{X}(h)]' \), \( h = 1, \ldots, u \). Namely we will have

\[
\begin{align*}
M(0) &= D(J_{a(1)}, \ldots, J_{a(h)}) \\
M(h) &= D(I_{a(1)}, \ldots, I_{a(h)}, J_{a(h+1)}, \ldots, J_{a(u)}), h = 1, \ldots, u - 1 \\
M(u) &= D(I_{a(1)}, \ldots, I_{a(u)})
\end{align*}
\]

(3.12)

The matrices in \( pb[ \times_{h=1}^{u} \mathcal{A}(a(h))] \) are

\[
\begin{align*}
Q_1(h) &= D(B_{1,1}(h), \ldots, B_{1,u}(h)), h = 1, \ldots, u \\
Q_2(h) &= D(B_{2,1}(h), \ldots, B_{2,u}(h)), h = 1, \ldots, u
\end{align*}
\]

(3.13)

with

\[
\begin{align*}
B_{1,h^*}(h) &= B_{2,h^*}(h) = 0_{a(h^*) \times a(h^*)}, h^* \neq h, h = 1, \ldots, u \\
B_{1,h}(h) &= \frac{1}{\alpha(h)} J_{a(h)}, h = 1, \ldots, u \\
B_{2,h}(h) &= K_{a(h)}, h = 1, \ldots, u
\end{align*}
\]

(3.14)
Since

\[(3.15) \quad \sum_{h=1}^{u} [Q_1(h) + Q_2(h)] = I_n,\]

with \(n = \sum_{h=1}^{u} a(h)\) the commutative Jordan algebra will be complete. We have also

\[
M(0) = \sum_{k=1}^{u} a(k) Q_1(k)
\]

\[
M(h) = \sum_{k=1}^{h} [Q_1(k) + Q_2(k)] + \sum_{k=h+1}^{u} a(k) Q_1(k), \quad h = 1, \ldots, u-1.
\]

\[
M(u) = \sum_{k=1}^{u} [Q_1(k) + Q_2(k)] = I_n
\]

Thus

\[
V = \sum_{h=1}^{u} \sigma^2 \left[ \sum_{k=1}^{h} [Q_1(k) + Q_2(k)] + \sum_{k=h+1}^{u} a(k) Q_1(k) \right]
\]

\[
= \sum_{h=1}^{u} \gamma_1(h) Q_1(h) + \sum_{h=1}^{u} \gamma_2(h) Q_2(h),
\]

where

\[
\gamma_1(h) = \sum_{k=1}^{h-1} a(h) \sigma^2(k) + \sum_{k=h}^{u} \sigma^2(k)
\]

\[
\gamma_2(h) = \sum_{k=h}^{u} \sigma^2(k).
\]
Moreover, $p_{\mathcal{A}^b \times_{h=1}^u \mathcal{A} (a (h))}^\frac{1}{2}$ will be constituted by the

\[
\begin{cases}
A_1 (h) = [C_{1,1} (h), \ldots, C_{1,u} (h)], & h = 1, \ldots, u \\
A_2 (h) = [C_{2,1} (h), \ldots, C_{2,u} (h)], & h = 1, \ldots, u ,
\end{cases}
\]

with

\[
\begin{cases}
C_{1,h^*} (h) = [0^{a(h^*)}]', & h \neq h^* \\
C_{2,h^*} (h) = 0_{a(h)-1 \times a(h^*)}, & h \neq h^* \\
C_{1,h} (h) = \frac{1}{\sqrt{a(h)}} [1^{a(h)}]', & h = 1, \ldots, u \\
C_{2,h} (h) = T_{a(h)}, & h = 1, \ldots, u
\end{cases}
\]

We thus have

\[
\begin{cases}
g_1 (h) = \text{rank} [A_1 (h)] = \text{rank} [Q_1 (h)] = 1, & h = 1, \ldots, u \\
g_2 (h) = \text{rank} [A_2 (h)] = \text{rank} [Q_2 (h)] = a (h) - 1, & h = 1, \ldots, u
\end{cases}
\]

3.2. Inference

Assuming that $\boldsymbol{y}$ is normal with mean vector $\boldsymbol{\mu}$ and variance-covariance matrix $\boldsymbol{V}$, we put $\boldsymbol{y} \sim \mathcal{N} (\boldsymbol{\mu}, \boldsymbol{V})$. Thus the

\[
\tilde{\eta}_l (h) = A_l (h) \boldsymbol{y}, \; l = 1, 2; \; h = 1, \ldots, u
\]

will be $\mathcal{N} (\eta_l (h), \gamma_l (h) I_{g_l (h)}), \; l = 1, 2, \; h = 1, \ldots, u$, with
(3.23) \[ \eta_l(h) = A_l(h) \mu, \quad l = 1, 2; \quad h = 1, \ldots, u. \]

It is easy to see that \( \eta_2(h) = 0^{g_2(h)}, \quad h = 1, \ldots, u, \) and that the cross of covariance matrices of the \( \tilde{\eta}_l(h), \quad l = 1, 2, \quad h = 1, \ldots, u, \) are null so these vectors will be independent.

We will center inference on the variance components using the fact that the \( S(h) = \|\tilde{\eta}_2(h)\|^2, \quad h = 1, \ldots, u \) are the products by \( \gamma_2(h), \quad h = 1, \ldots, u \) of independent central chi-squares with \( g_2(h), \quad h = 1, \ldots, u, \) degrees of freedom. Thus we have the unbiased estimators

(3.24) \[ \tilde{\gamma}_2(h) = \frac{S(h)}{g_2(h)}, \quad h = 1, \ldots, u \]

from which we get

(3.25) \[ \begin{cases} \tilde{\sigma}^2(u) = \tilde{\gamma}_2(u) \\
\tilde{\sigma}^2(h) = \tilde{\gamma}_2(h) - \tilde{\gamma}_2(h+1), \quad h = 1, \ldots, u - 1 \end{cases} \]

The possibility of negative estimators has been considered by many authors (see, for example Nelder, 1954). The main inference to be had when we get \( \tilde{\sigma}^2(h) < 0 \) is that \( \sigma^2(h) \) must be null or very small.

Moreover we have, as we saw,

(3.26) \[ V = \sum_{h=1}^{u} \sum_{l=1}^{2} \gamma_l(h) Q_l(h) \]

so

(3.27) \[ \begin{cases} V^{-1} = \sum_{h=1}^{u} \sum_{l=1}^{2} [\gamma_l(h)]^{-1} Q_l(h) \\
\det(V) = \prod_{h=1}^{u} \prod_{l=1}^{2} [\gamma_l(h)]^{g_l(h)} \end{cases} \]

and since that
\[(y - \mu)^T \mathbf{V}^{-1} (y - \mu) = \sum_{h=1}^{u} \sum_{l=1}^{2} \left( y - \mu \right)^T \left[ \mathbf{A}_l (h) \right]' \left[ \mathbf{A}_l (h) \right] (y - \mu) \gamma_l (h) \]

\[= \sum_{h=1}^{u} \frac{\| \bar{\eta}_1 (h) - \eta_1 (h) \|^2}{\gamma_1 (h)} + \sum_{h=1}^{u} \frac{S (h)}{\gamma_2 (h)} \]

the density of \(y\) will be

\[n (y) = e^{-\frac{1}{2} \left[ \sum_{h=1}^{u} \frac{\| \bar{\eta}_1 (h) - \eta_1 (h) \|^2}{\gamma_1 (h)} + \sum_{h=1}^{u} \frac{S (h)}{\gamma_2 (h)} \right]} \frac{1}{(2\pi)^{u} \prod_{h=1}^{u} \prod_{l=1}^{2} \left[ \gamma_l (h) \right]^{g_l (h)}} \]

We may now establish

**Proposition 2.** The \(\bar{\eta}_1 (h)\) and \(S (h)\), \(h = 1, \ldots, u\) are sufficient and complete statistics. The \(\bar{\gamma}_2 (h)\) and \(\bar{\sigma}_2 (h)\), \(h = 1, \ldots, u\), are UMVUE.

**Proof.** Using the factorization theorem we see that the \(\bar{\eta}_1 (h)\) and \(S (h)\), \(h = 1, \ldots, u\) are sufficient. These statistics are complete because the normal distribution belongs to the exponential family and, for these models, the parameter space contains open sets (see Silvey, 1975). The last part of the thesis is now a direct consequence of the Blackwell-Lehman-Scheffé theorem.

For the \(\gamma_2 (h)\), \(h = 1, \ldots, u\) we get \(1 - q\) level confidence intervals:

\[
\left\{ \begin{array}{c}
0; \\
S (h) \frac{1}{x_{q,g_2(h)}}
\end{array} \right\}
\]

\[
\left\{ \begin{array}{c}
S (h) \frac{1}{x_{1-g_2(h)}}; \\
S (h) \frac{1}{x_{2-g_2(h)}}
\end{array} \right\}
\]

\[
\left\{ \begin{array}{c}
S (h) \frac{1}{x_{1-q,g_2(h)}}; \\
+\infty
\end{array} \right\}
\]
with \( x_{p,g} \) the quantile for probability \( p \) of a central chi-square with \( g \) degrees of freedom.

These confidence intervals may be used to derive, through duality, \( q \) level tests for

\[
H_0(h) : \gamma_2(h) = \gamma_{2,0}(h), \quad h = 1, \ldots, u.
\]

The tested hypothesis is rejected when the \( 1 - q \) level confidence interval does not contain \( \gamma_{2,0}(h), \quad h = 1, \ldots, u \). When the first \( \text{[second; third]} \) confidence interval is used the corresponding tests will be left one-sided \( \text{[two-sided; right one-sided]} \).

The

\[
Z(h) = \frac{g_2(h + 1)}{g_2(h)} \frac{S(h)}{S(h + 1)}, \quad h = 1, \ldots, u - 1
\]

will be the product by

\[
v(h) = \frac{\gamma_2(h)}{\gamma_2(h + 1)}, \quad h = 1, \ldots, u - 1
\]

of a variable with a central \( F \) distribution with \( g_2(h) \) and \( g_2(h + 1) \) degrees of freedom. With \( f_{p,g,g'} \) the quantile for probability \( p \) of the central \( F \) distribution with \( g \) and \( g' \) degrees of freedom we get the \( 1 - q \) confidence level intervals:

\[
(3.34) \quad \left[ \begin{array}{c}
0; \\
\frac{Z(h)}{f_{q,g_2(h),g_2(h+1)}} \\
\frac{Z(h)}{f_{1-q,g_2(h),g_2(h+1)}}, +\infty \\
\end{array} \right]
\]

for \( v(h), \quad h = 1, \ldots, u - 1 \).
These confidence intervals may be used to derive, through duality, $q$ level tests for

$$(3.35) \quad H_0(h) : v(h) = v_0(h), \ h = 1, \ldots, u - 1.$$ 

The tested hypothesis is rejected when the $1 - q$ level confidence interval does not contain $v_0(h), \ h = 1, \ldots, u - 1$. When the first \second; \third confidence interval is used the corresponding tests will be left one-sided \two-sided; \right one-sided.

4. Final Comments

In balanced nesting we are forced to divide repeatedly the plots and we have few degrees of freedom for the first levels. This decrease of plot size leads to new shortcomings of these designs. So the step nesting designs turned out to be a valid alternative for the balanced nested designs because we can work with fewer observations and the amount of information for the different factors is more evenly distributed. As in a practice experiment, the carry cost is, many times, a decisive factor, so the step nesting design is a strong alternative to the balanced nested design.

It is quite interesting to point out that the models with step nesting are important because they are orthogonal but not balanced.

References


Received 5 February 2010