Adjusted Orthogonality Properties in Multiway Block Designs

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SUMMARY

We show that adjusted orthogonality properties are necessary and sufficient for a multiway block design to be uniformly optimal for estimating the treatment contrasts.

Some key words: Determining blocking factor; experimental design; multiway C-matrix; treatment contrasts.

AMS 1980 Subject Classification: 62K05, 62K10.

1. Introduction

We consider a design D with m blocking factors. We assume that the model has additive fixed effects and no interactions, and is given by

$$y_{ij_1\ldots j_m t} = \alpha_i + \gamma_{1j_1} + \cdots + \gamma_{mj_m} + e_{ij_1\ldots j_m t},$$

with $i = 1, \ldots, a$, and $j_k = 1, \ldots, b_k$ for $k = 1, \ldots, m$, and $t = 1, \ldots, n_{ij_1\ldots j_m}$.

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level j_k of the kth blocking factor. The observational errors $e_{ij_1\ldots j_m t}$ are assumed to be uncorrelated, with mean zero and variance $\sigma^2 > 0$.

In matrix notation the model turns into

$$y = U\alpha + \sum_{k=1}^{m} Z_k \gamma_k + e,$$

with $n = \sum_{i,j_1,\ldots,j_m} n_{ij_1\ldots j_m}$. Let 1_n denote the $n \times 1$ vector of ones. The design matrices U and Z_k are binary $n \times a$ and $n \times b_k$ matrices, respectively, and satisfy $U1_a = Z_k 1_{b_k} = 1_n$. They are related to the incidence matrices N_k between treatments and blocking factor k, and $N_{k\ell}$ between blocking factors k and ℓ, for $k, \ell = 1, \ldots, m$ with $k \neq \ell$, through

$$N_k = U'Z_k, \qquad N_{k\ell} = Z_k' Z_\ell,$$

where the superscript $'$ denotes transposition. Moreover, we designate by $\Delta_k = Z_k' Z_k$ the diagonal matrix with diagonal elements equal to the replication number of the levels of blocking factor k, for $k = 1, \ldots, m$.

Our interest concentrates on the *treatment contrasts*

$$(\alpha_1 - \overline{\alpha}., \ldots, \alpha_a - \overline{\alpha}.)',$$

with $\overline{\alpha}. = \sum_i \alpha_i / a$, while the effects γ_{kj_k} are considered as nuisance parameters. As usual the information matrix for the treatment contrasts is denoted by C, we call C the *contrast information matrix*. We are also interested in the matrix

$$C_k = \Delta_0 - N_k \Delta_k^{-1} N_k',$$

the contrast information matrix of the simple block design for treatments and factor k only, where Δ_0 is the diagonal matrix of treatment replications. Pukelsheim & Titterington (1986), eq. (4), use the formula

$$C = C_k - B_k,$$

where the matrix B_k is nonnegative definite. This shows that the contrast information matrix in an m-way block design, C, may be obtained from the contrast information matrix in a simple block design, C_k, by subtracting a penalty term B_k due to entertaining the nuisance parameters that come with the other blocking factors $\ell \neq k$.

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is uniformly optimal for the treatment contrasts, among the designs that lead to the same "marginal" contrast information matrix C_k.

Pukelsheim & Titterington (1986), page 263 gave a sufficient condition for the penalty term B_k to vanish. However, that condition fails to be necessary. In the present note we provide a necessary and sufficient condition for the equality $C = C_k$.

2. Necessary and sufficient condition

Out of the existing blocking factors $1, \ldots, m$ we consider a fixed blocking factor k.

THEOREM 1. *An m-way block design satisfies*

$$C = C_k$$

if and only if the treatments and the blocking factors $\ell \neq k$ are orthogonal after adjusting for blocking factor k, that is,

$$N_k \Delta_k^{-1} N_{k\ell} = N_\ell$$

for all $\ell = 1, \ldots, m$ with $\ell \neq k$.

Proof. Without loss of generality we choose $k = 1$. For a matrix A let $\mathcal{R}(A)$ designate the range (column space) of A, and denote by P_A and Q_A the orthogonal projectors onto $\mathcal{R}(A)$ and onto the orthogonal complement of $\mathcal{R}(A)$, respectively.

We find it convenient to base the analysis on the representation

$$C = U' Q_{(Z_1, \ldots, Z_m)} U, \tag{1}$$

where $(Z_1, \ldots, Z_m)$ denotes the partitioned matrix comprising the matrices $Z_1, \ldots, Z_m$; see Hedayat & Majumdar (1985), page 698. From the decomposition of $\mathcal{R}(Z_1, \ldots, Z_m)$ into the orthogonal direct sum of $\mathcal{R}(Z_1)$ and
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$\mathcal{R}(Q_{Z_1}(Z_2, \ldots, Z_m))$ it follows that

$$Q_{(Z_1, \ldots, Z_m)} = I_n - (P_{Z_1} + P_{(S_2, \ldots, S_m)}) = Q_{Z_1} - P_{(S_2, \ldots, S_m)}, \tag{2}$$

where $S_\ell = Q_{Z_1} Z_\ell$ for $\ell \geq 2$.

Substitution of (2) into (1) yields $C = C_1 - U' P_{(S_2, \ldots, S_m)} U$. This shows that $C = C_1$ if and only if $U' S_\ell = 0$ for $\ell \geq 2$. With $S_\ell = Q_{Z_1} Z_\ell$, the latter becomes

$$U' Q_{Z_1} Z_\ell = 0. \tag{3}$$

□

Adjusted orthogonality was introduced by Eccleston & Russell (1975); it is also known as *strict orthogonality*. Its relationships to another, weaker version of orthogonality is studied by Khatri & Shah (1986), Styan (1986), and Baksalary & Styan (1991). As predicted by Eccleston & Russell (1975), page 341, the concept of adjusted orthogonality proves to be *useful and reasonable in many situations*. Their Theorem 1 (1975) page 343, compares connectedness of a design D, with m blocking factors, and the design D_k, with only the kth blocking factor, that is, it concentrates on whether C has rank $a-1$ when C_k has rank $a-1$. The conclusion of our Theorem 1 is considerably stronger, in that we assert equality of the matrices themselves.

COROLLARY 1. *For a two-way block design D with treatments orthogonal to rows after adjusting for columns, D has the same subspace of estimable treatment contrasts as the treatment–column one-way block design D_2. In particular, D is connected if and only if D_2 is connected.*

Proof. By Theorem 1 the matrices C and C_2 are equal, hence so are their ranges which represent the corresponding subspaces of estimable treatment contrasts. □

In terms of design optimality we have the following corollary. Eccleston & Kiefer (1981) study optimality criteria that are real-valued. In contrast we here apply the notion of *uniform optimality* of Kurotschka (1971) which refers to the usual (Loewner) matrix ordering. This is a strong optimality concept, and the present situation provides one of the rare circumstances where it can be brought to bear.

COROLLARY 2. *An m-way block design such that treatments are orthogonal to blocking factors $\ell \neq k$ after adjusting for factor k is uniformly optimal for the treatment contrasts, among the designs with incidence matrix N_k between treatments and blocking factor k.*

Proof. The candidate design has contrast information matrix $C = C_k$, by Theorem 1. Every competing design with contrast information matrix $\widetilde{C}$, say, satisfies $\widetilde{C} = C_k - \widetilde{B}_k \leq C_k = C$. □

Pukelsheim & Titterington (1986) page 263, introduced the concept of a *determining blocking factor* k by the condition that just a single level $j_\ell(j_k)$ of each blocking factor $\ell \neq k$ appears with level j_k of factor k, for all $j_k = 1, \ldots, b_k$. In terms of the design matrices $Z_1, \ldots, Z_m$ this property is equivalent

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an m-way block design with a determining blocking factor k satisfies $C = C_k$. However, the present result says more, in that it provides an interpretation of how far the concept of a determining blocking factor is "necessary".

COROLLARY 3. *An m-way block design satisfies $C = C_k$ irrespective of the treatment design matrix U if and only if blocking factor k is a determining factor.*

Proof. The adjusted orthogonality condition (3) holds true for all treatment design matrices U if and only if $Q_{Z_1} Z_t = 0$. □

3. EXAMPLES

There are several examples of designs having the property mentioned in Theorem 1. None of the designs given below has a determining factor. We present two examples of two-way block designs, $m = 2$, with rows and columns as blocking factors, and one example of a three-way block design. The contrast information matrices turn out to be proportional to the $a \times a$ *orthodiagonal projector*

$$K_a = I_a - \frac{1}{a} 1_a 1_a'.$$

I. An interesting illustration is the design for 12 observations on 3 treatments in a 4×4 blocking system, with allocation table

$$\begin{array}{cccc} 1 & 2 & 3 & - \\ 2 & 3 & - & 1 \\ 3 & - & 1 & 2 \\ - & 1 & 2 & 3 \end{array},$$

$$\begin{array}{cccc} - & 1 & 2 & 3 \end{array}$$

where the integers denote treatment levels. This design has $C = C_1 = C_2 = 4K_3$

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$$N_1 = N_2 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} = 1_3 1_4'.$$

In the terminology of Pukelsheim (1986), page 340, this design is a variety–factor product design.

II. More generally, two-way block designs with the property $C = C_2$ can be whose rows and columns are orthogonal after adjusting for treatments. The following example is a design for 36 observations on 12 treatments in a 4×9 blocking system, with allocation table

$$\begin{array}{ccccccccc}
1 & 11 & 3 & 5 & 6 & 10 & 4 & 9 & 7 \\
2 & 5 & 4 & 6 & 7 & 8 & 11 & 10 & 12 \\
4 & 3 & 12 & 8 & 2 & 7 & 9 & 5 & 1 \\
10 & 2 & 6 & 1 & 9 & 3 & 8 & 12 & 11
\end{array},$$

see Table 2 of Anderson & Eccleston (1985), page 134. By interchanging treatments and columns and permuting the columns so as to obtain a nice pattern we get a design for 36 observations on 9 treatments in a 4×12 blocking system,

$$\begin{array}{cccccccccccc}
- & 3 & 5 & 7 & - & 8 & 6 & 4 & - & 1 & 2 & 9 \\
1 & - & 4 & 3 & 6 & - & 8 & 2 & 9 & - & 7 & 5 \\
5 & 2 & - & 1 & 4 & 7 & - & 8 & 3 & 9 & - & 6 \\
2 & 6 & 3 & - & 7 & 5 & 1 & - & 8 & 4 & 9 & -
\end{array}.$$

This design satisfies $N_2\Delta_2^{-1}N_{21} = N_1$ and $N_1\Delta_1^{-1}N_{12} \neq N_2$. By Theorem 1 it then fulfills $C = C_2 \leq C_1$. Indeed, we obtain $C_2 = 3K_9 \leq 4K_9 = C_1$. According to Corollary 2 the design is optimal among all two-way block designs with treatment–column incidence matrix

$$N_2 = \begin{pmatrix}
1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1
\end{pmatrix}.$$

III. The final illustration is an example with $m = 3$ blocking factors, obtained as a modification of the example given by Eccleston & Russell (1977), page 344.

III. The final illustration is an example with $m = 3$ blocking factors, obtained as a modification of the example given by Eccleston & Russell (1977), page 344. This is a design for 16 observations on 4 treatments in a $4 \times 8 \times 2$ blocking system, with row–column pattern

$$\begin{array}{cccccccc}
1 & 2 & - & - & - & - & - & - \\
2 & 1 & - & - & - & - & - & - \\
- & - & 3 & 4 & - & - & - & - \\
- & - & 4 & 3 & - & - & - & -
\end{array}, \qquad
\begin{array}{cccccccc}
- & - & - & - & 1 & 2 & - & - \\
- & - & - & - & 2 & 1 & - & - \\
- & - & - & - & - & - & 3 & 4 \\
- & - & - & - & - & - & 4 & 3
\end{array},$$

in layers 1 and 2, respectively. Application of Theorem 1 shows that $C = C_1 =$

$4(I_2 \otimes K_2) + 2(K_2 \otimes 1_2 1_2')$. By Corollary 2, optimality of the design extends over the three-way block designs with treatment–row incidence matrix

$$N_1 = \begin{pmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{pmatrix},$$

as well as over the three-way block designs with treatment–column incidence matrix

$$N_2 = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

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Preface

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