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Efficient Block Designs for Estimating Conditional Main Effects Contrasts

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SUMMARY

Designs consisting of the Kronecker product of two balanced incomplete block designs are considered for estimating conditional main effects contrasts in a two-factor experiment. Conditional main effects contrasts are pairwise differences of treatment combinations in which the level of one factor is kept fixed. It is shown that the designs under consideration are highly efficient for estimating these contrasts, and that Kronecker products of other standard designs can also yield efficient designs for this problem, as can standard incomplete block designs.

Key words : A-optimality, Balanced incomplete block design, Conditional main effect contrasts, Factorial experiment, Kronecker product design, Simple effects.

1. *Introduction*

Consider a factorial experiment involving two factors A and B arranged as a block design. Factor A has $v_1 \geq 2$ levels labelled $1, \ldots, v_1$ and factor B has $v_2 \geq 2$ levels labelled $1, \ldots, v_2$. Without loss of generality, we assume $v_1 \geq v_2$ throughout the paper. A treatment consists of a combination of the levels of A and B, denoted by (pq) if level p of A is present and level q of B is present. Treatments are to be given to bk experimental units in b blocks of size k and a response is to be measured on each unit. To model the response, we use the usual intra-block model

$$Y = Z\beta + X\tau + \varepsilon \tag{1.1}$$

where Y is a random vector of N observations, ε is a random vector of independent identically distributed error variables, and Z and X are design matrices corresponding to parameter vectors $\beta = \{\mu, \beta_1, \beta_2 \ldots \beta_b\}$ and $\tau = \{\tau_{11}, \tau_{12}, \ldots, \tau_{1v_2}, \tau_{21}, \tau_{22}, \ldots, \tau_{2v_2}, \cdots, \tau_{v_1v_2}\}$, where μ is a constant, β_j represents the effect of the jth block, and τ_{pq} represents the effect of treatment (pq).

We assume that the researcher is interested in comparing treatments in which the level of one factor is held fixed, that is, in comparing treatment (pq) with treatment (ps) and/or with treatment (hq). In terms of treatment effects, the researcher is interested in estimating contrasts of the form $\tau_{pq} - \tau_{ps}$ or $\tau_{pq} - \tau_{hq}$ ($s \neq q$, $h \neq p$). There are $v_1 v_2 (v_1 + v_2 - 2)/2$ distinct contrasts of this type and we shall call them conditional main effect contrasts. In the behavioral sciences, these contrasts are often called simple effects (see, for example, Maxwell and Delaney [7], Chapter 7). Our goal is to find designs for model (1.1) which are optimal or efficient for estimating the set of conditional main effect contrasts.

To this end, let c_1 denote the vector of the $v_1 v_2 (v_2 - 1)/2$ conditional main effect contrasts with a fixed level of the first factor, ordered as

$$c_1 = (\tau_{11} - \tau_{12}, \tau_{11} - \tau_{13}, \dots, \tau_{11} - \tau_{1v_2}, \tau_{12} - \tau_{13}, \tau_{12} - \tau_{14}, \dots, \tau_{12} - \tau_{1v_2},$$
$$\tau_{13} - \tau_{14}, \dots, \tau_{1(v_2-1)} - \tau_{1v_2}, \tau_{21} - \tau_{22}, \tau_{21} - \tau_{23}, \dots, \tau_{v_1(v_2-1)} - \tau_{v_1 v_2})' \tag{1.2}$$

where " ′ " denotes transpose. Similarly, let c_2 denote the vector of the $v_1 v_2 (v_1 - 1)/2$ conditional main effect contrasts with a fixed level of the second factor, ordered as

$$c_2 = (\tau_{11} - \tau_{21}, \tau_{11} - \tau_{31}, \dots, \tau_{11} - \tau_{v_1 1}, \tau_{21} - \tau_{31}, \tau_{21} - \tau_{41}, \dots, \tau_{21} - \tau_{v_1 1},$$
$$\tau_{31} - \tau_{41}, \dots, \tau_{(v_1-1)1} - \tau_{v_1 1}, \tau_{12} - \tau_{22}, \tau_{12} - \tau_{32}, \dots, \tau_{(v_1-1)v_2} - \tau_{v_1 v_2})' \tag{1.3}$$

Let H be the matrix satisfying $c = H\tau$, where $c = (c_1', c_2')'$. A design d for model (1.1) is a specification of the treatments (pq) which are to be used in each block and can be represented by its incidence matrix N_d, a matrix with $v_1 v_2$ rows labelled by the treatments $(11), (12), \dots, (v_1 v_2)$ and with b columns and whose entry in row (pq) and in column h is the number of times treatment (pq) appears in block h. Let $D(v_1 v_2, b, k, r)$ be the class of connected block designs for $v_1 v_2$ treatments replicated r times and with b blocks of size k. The intra-block information matrix for a design d in $D(v_1 v_2, b, k, r)$ is

$$C_d = r I_{v_1 v_2} - (1/k) N_d N_d' \tag{1.4}$$

where $I_{v_1 v_2}$ is the identity matrix of order $v_1 v_2$.

We seek designs $d \in D(v_1v_2, b, k, r)$ which minimize the average variance of the least squares estimators of all $v_1v_2(v_1+v_2-2)/2$ conditional main effect contrasts which is equivalent to minimizing $tr(HC_d^- H')$ over all designs $d \in D(v_1v_2, b, k, r)$, where tr denotes trace. Designs which minimize $tr(HC_d^- H')$ are called A-optimal for estimating conditional main effect contrasts. Designs which 'nearly' minimize $tr(HC_d^- H')$ are called A-efficient for estimating conditional main effect contrasts.

2. *Optimal Kronecker Product Designs*

We note that the conditional main effect contrasts in the vector c_1 of (1.2) are contrasts in the levels of the second factor. Similarly, contrasts in c_2 of (1.3) are contrasts in the levels of the first factor. Consequently, it is natural to suppose that designs efficient for estimating the usual main effect contrasts will also be efficient for estimating simple effects.

All designs d having orthogonal factorial structure are efficiency consistent (Lewis and Dean [5]). This property ensures that the efficiency of each main effect in the design d is the same as that in the subdesign d_i obtained from d by ignoring all factors except for the ith. Such designs include the Kronecker product designs of Vartak [9] and the generalizations of Mukherjee [8] and Gupta [2]. The standard Kronecker product designs of Vartak [9] defined below, form the natural class for our design problem.

Definition 2.1. A Kronecker product design d is a design in $D(v_1v_2, b_1b_2, k_1k_2, r_1r_2)$ whose incidence matrix N_d is formed from the Kronecker product of the incidence matrices N_1 and N_2 of two block designs $d_1 \in D(v_1, b_1, k_1, r_1)$ and $d_2 \in D(v_2, b_2, k_2, r_2)$, that is $N_d = N_1 \otimes N_2$.

The information matrix for a Kronecker product design $d \in D(v_1v_2, b_1b_2, k_1k_2, r_1r_2)$ is

$$C_d = r_1r_2 I_{v_1v_2} - (1/k_1k_2) N_1N_1' \otimes N_2N_2' \qquad (2.1)$$

Due to the efficiency consistency of such a design, if N_1 and N_2 are the incidence matrices for complete block or balanced incomplete block designs, the Kronecker product design d is optimal in the sense of minimizing the average variance of the least squares estimators of all pairwise comparisons in the levels of each main effect, that is, the design is A-optimal for these contrasts. We call such Kronecker product designs BIB-Kronecker product designs. We may like to conjecture that BIB-Kronecker product designs would be optimal for estimating the set of conditional main effect contrasts. However, this is not necessarily the case as the following example illustrates.

Example 2.1. Consider balanced incomplete block designs $d_1 \in D(5, 10, 2, 4)$ and $d_2 \in D(2, 3, 2, 3)$. Let $d \in D(10, 30, 4, 12)$ be the BIB-Kronecker product design based on d_1 and d_2. Let d^* be a balanced incomplete block design in $D(10, 30, 4, 12)$. The efficiency of d^* relative to that of d for estimating the conditional main effect contrasts can be shown to be 1.033.

Example 2.1 might suggest that balanced incomplete block designs might form a better class of designs for our problem. However, this is not the case either, as shown by Example 2.2.

Example 2.2. Consider balanced incomplete block designs $d_1 = d_2$ in $D(5, 10, 2, 4)$. Let $d \in D(25, 100, 4, 16)$ be the BIB-Kronecker product design based on d_1 and d_2. Let d^* be a balanced incomplete block design in $D(25, 100, 4, 16)$. The efficiency of d^* relative to that of d for estimating the conditional main effect contrasts is 0.977.

Even though, as shown by Example 2.1, BIB-Kronecker product designs may not be optimal for our problem, they form a natural class of study as shown below.

Theorem 2.1 (Kao *et al.* [4]). Let $\mathcal{M}$ be the set of all symmetric, non-negative definite matrices of size v, with row sums zero and rank $v-1$. (This includes the set of all information matrices (1.4) for designs for model (1.1). Let H be as defined in Section 1, and let $1, o_1, \ldots, o_{v-1}$ be a set of orthonormal eigenvectors of $H'H$ with corresponding eigenvalues $0, \theta_1, \ldots, \theta_{v-1}$. Then

$$\operatorname{tr}(HM^{*-}H') = \min\{\operatorname{tr}(HM^{-}H'), M \in \mathcal{M}\}$$

$$\text{if and only if } M^* = \alpha \sum_{i=1}^{v_1 v_2 - 1} \sqrt{\theta_i}\, o_i o'_i$$

where α is a constant such that trace (M^*) is equal to the maximum trace of all information matrices C_d; that is $\alpha = b(k-1)/\Sigma\sqrt{\theta_i}$ for a binary design in $D(v, b, k, r)$.

For the conditional main effect contrasts, H_T, it can be verified that

$$H'H = (\upsilon_1 + \upsilon_2)\, I_{\upsilon_1} \otimes I_{\upsilon_2} - I_{\upsilon_1} \otimes J_{\upsilon_2} - J_{\upsilon_1} \otimes I_{\upsilon_2} \qquad (2.2)$$

and a set of orthonormal eigenvectors and corresponding eigenvalues of H′H are

eigenvector $(v_1v_2)^{-1/2}\, 1_{v_1v_2}$ with eigenvalue 0

eigenvectors $\{ v_1^{-1/2} 1_{v_1} \otimes w_j, j = 1, \ldots, v_2 - 1 \}$ with eigenvalue v_2

eigenvectors $\{ u_i \otimes v_2^{-1/2}\, 1_{v_2},\ i = 1, \ldots, v_1 - 1 \}$ with eigenvalue v_1

eigenvectors $\{ u_i \otimes w_j,\ i = 1, \ldots, v_1 - 1,\ j = 1, \ldots, v_2 - 1 \}$

with eigenvalue $v_1 + v_2$ (2.3)

Now $\{ v_1^{-1/2}\, 1_{v_1}, u_1, u_2 \ldots, u_{v_1 - 1} \}$ is a set of orthonormal $v_1 \times 1$ vectors and $\{ v_2^{-1/2}\, 1_{v_2}, w_1, w_2, \ldots, w_{v_2 - 1} \}$ is a set of orthonormal $v_2 \times 1$ vectors. Notice that the set of orthonormal eigenvectors (2.3) of H′H is also a set of orthonormal eigenvectors for C_d in (2.1). In order that the eigenvalues of C_d have the same multiplicities as those of H′H, d is required to be a BIB- Kronecker product design, based on d_1 and d_2, where d_i has v_i treatments replicated r_i times, b_i blocks of size $k_i \geq 2$, and $\lambda_i = r_i (k_i - 1) / (v_i - 1), i = 1, 2$. Using the definition of Lewis and Gerami [6], BIB-Kronecker product designs are strongly aligned with H′H. By Theorem 2.1, a sufficient condition for a BIB- Kronecker product design d to be an A-optimal design for model (1.1) is that there must exist α such that

$$\begin{aligned} \alpha\sqrt{v_2} &= r_1 \lambda_2 v_2/k_2 \\ \alpha \sqrt{v_1} &= r_2\lambda_1 v_1 / k_1 \\ \alpha \sqrt{v_1 + v_2} &= [r_1r_2 - (r_1 - \lambda_1)(r_2 - \lambda_2) / k_1 k_2] \end{aligned} \tag{2.4}$$

One can show that in order for a design to satisfy (2.4), k_1 and k_2 must both be 2. Since no known BIB designs with these block sizes satisfy these equations, no BIB-Kronecker product design has information matrix equal to M* of Theorem 2.1. However, since the structure of the information matrices of BIB-Kronecker product designs is "close" to that of M*, these designs provide a source of highly efficient designs for estimating conditional main effect contrasts. A similar approach was suggested independently by Lewis and Gerami [6]. In the next section, we show that BIB-Kronecker product designs are highly efficient in general, and in Sections 4 and 5 we look at generalizations of this class.

3. *Efficiency of BIB-Kronecker Product Designs*

We define the efficiency of a BIB-Kronecker product design for estimating a set of contrasts $H\tau$ as follows :

Definition 3.1. Let $H\tau$ be a vector of contrasts, then the efficiency e_d of design $d \in D(v_1 v_2, b_1 b_2, k_1 k_2, r_1 r_2)$ is defined as

$$e_d = \frac{B(H)}{tr(HC_d^- H')}$$

where B(H) is the lower bound given by Theorem 2.1 for $tr(HC_d^- H')$ over $D(v_1v_2, b_1b_2, k_1k_2, r_1r_2)$, and coincides with the bound obtained by Gerami and Lewis [1], that is $B(H) = \dfrac{(\Sigma \sqrt{\theta_i})^2}{b_1b_2(k_1k_2 - 1)}$, where $\theta_1, \theta_2, \ldots, \theta_{v_1v_2}$ are the eigenvalues of $H'H$.

From (2.3), and the fact that $b_1b_2 = r_1r_2v_1v_2/k_1k_2$, it follows that, for the conditional main effect contrasts $H\tau$ defined in Section 1,

$$B(H) = \frac{((v_1 - 1)(v_2 - 1)\sqrt{v_1 + v_2} + (v_1 - 1)\sqrt{v_1} + (v_2 - 1)\sqrt{v_2})^2}{b_1b_2(k_1k_2 - 1)} \tag{3.1}$$

If d is a BIB-Kronecker product design as in Section 2 then, using (2.2) and (2.3), and the fact that $[r_1r_2 - (r_1 - \lambda_1)(r_2 - \lambda_1)/k_1k_2] = [r_1k_1v_2\lambda_2 + r_2k_2v_1\lambda_1 - v_1v_2\lambda_1\lambda_2]/k_1k_2$, it follows that

$$tr(HC_d^- H') = tr(C_d^- H'H)$$

$$= \frac{(v_1 - 1)(v_2 - 1)(v_1 + v_2)k_1k_2}{r_1k_1v_2\lambda_2 + r_2k_2v_1\lambda_1 - v_1v_2\lambda_1\lambda_2} + \frac{k_1(v_1 - 1)}{r_2\lambda_1} + \frac{k_2(v_2 - 1)}{r_1\lambda_2} \tag{3.2}$$

Taking the ratio of (3.1) and (3.2) yields, after some straightforward algebra, the following theorem which expresses the efficiency of a BIB-Kronecker product design in terms of v_1, v_2, k_1, k_2 only.

Theorem 3.1. Let $H\tau$ be the set of conditional main effects contrasts defined in Section 1, and let $d \in D(v_1v_2, b_1b_2, k_1k_2, r_1r_2)$ be a BIB-Kronecker product design. The efficiency e_d of the design d is given by

$$e_d^{-1} = \frac{1}{B}(v_1+v_2)(v_1-1)(v_2-1)\,v_1v_2\,(1+z)^{-1} + \frac{v_1v_2(k_1k_2-1)}{B}\left[\frac{(v_1-1)(k_2-1)}{(v_2-1)k_2(k_1-1)} + \frac{(v_2-1)(k_1-1)}{(v_1-1)k_1(k_2-1)}\right] \tag{3.3}$$

where

$$B = ((v_1-1)(v_2-1)\sqrt{v_1+v_2} + (v_1-1)\sqrt{v_1} + (v_2-1)\sqrt{v_2})^2 \tag{3.4}$$

and

$$z = \left(\frac{1}{(v_1-1)(v_2-1)(k_1k_2-1)}\right)[(v_1-k_1)(k_2-1)+(v_2-1)(k_1-1)] \tag{3.5}$$

Corollary 3.1. Let $v_1 \geq v_2$. A lower bound, $L(e_d; v_1,v_2)$ on the efficiency e_d of a BIB-Kronecker product design $d \in D(v_1 v_2, b, k, r)$ is given by

$$L(e_d; v_1,v_2) = \frac{B}{v_1v_2}\left[\frac{(v_1-1)(v_2-1)(v_1+v_2)v_1v_2}{(v_1v_2+1)} + (v_1-1)^2 + (v_2-1)^2 + (v_1-1)(v_2-1)U_A\right]^{-1} \tag{3.6}$$

where B is defined in (3.4), and

$$U_A = \begin{cases} 1 & \text{if } v_1 = v_2 \\ \left(\dfrac{(v_1-1)}{v_2} + \dfrac{1}{2(v_1-1)}\right) & \text{if } v_1 > v_2 \end{cases}$$

A proof of the corollary can be found in Kao, Notz and Dean [3].

The bound $L(e_d; v_1, v_2)$ in (3.6) is a function of v_1 and v_2 only, and it is straightforward to show that as v_1 and v_2 tend to infinity with $v_1 \geq v_2$, $L(e_d; v_1, v_2)$ tends to 1.0. Thus, for large values of v_1 and v_2, BIB-Kronecker product designs are expected to be highly efficient. In fact, even for small values of v_1 and v_2, e_d is above 0.92. The values of e_d range from 0.9211 to 0.9999 over the values $8 \geq v_1 \geq v_2 \geq 2$, with the larger efficiencies obtained for the larger values of v_2.

4. *BIB Designs*

From Examples 2.1 and 2.2, we see that balanced incomplete block designs, when they exist, can provide an alternative source of efficient designs. We note that these are also strongly aligned with H'H. The efficiency, e_d, as defined in Definition 3.1, can be shown to be

$$e_d^{-1} = \frac{1}{B} v_1 v_2 (v_1 v_2 - 1)(v_1 + v_2 - 2)$$

where B is given in (3.4). As v_1 and v_2 tends to infinity with $v_1 \geq v_2$, this efficiency tends to 1.0.

5. *GD-Kronecker Product Designs*

For parameter values where balanced incomplete block designs do not exist, natural replacements might be a group divisible design with parameters $\lambda_{i1} = \lambda_{i2} \pm 1$, where λ_{i1} and λ_{i2} are the numbers of times that first and second associates, respectively, occur together in the same blocks of the design d_i, $i = 1, 2$.

Let d_i be a group divisible design with m_i groups of size n_i and with $v_i = m_i n_i$ treatments observed r_i times in b_i blocks of size k_i, $(i = 1,2)$ and with $\lambda_{i1} = \lambda_{i2} \pm 1$. The eigenvalues of $N_i N'_i$ are $r_i k_i$ with multiplicity $m_i (n_i - 1)$, and $r_i k_i - v_i \lambda_{i2}$ with multiplicity $m_i - 1$. Let d be a GD-Kronecker product design formed from the Kronecker product of two group divisible designs d_1 and d_2. The eigenvalues of the information matrix C_d in (2.1) of the GD-Kronecker product design are obtained from products of those of $N_1 N'_1$ and $N_2 N'_2$ and can be matched with corresponding eigenvalues of H'H in (2.2). An expression for $tr(HC_d^- H')$ similar to (3.2) can then be obtained for the GD-Kronecker product design and the efficiency can be calculated by comparing this value with B(H) as in Definition 3.1. In Table 1, we show through a number of examples, that GD-Kronecker product designs are highly efficient for estimating conditional main effects contrasts.

6. *Conclusions*

In this paper, we have considered three different classes of designs for estimating conditional main effect contrasts $H\tau$ and have shown them to be highly efficient. The motivation for studying these classes was as follows. Theorem 3.1 suggested the structure of the information matrix of the optimal design for this problem—the structure coinciding with that of a BIB-Kronecker product design. These designs are strongly aligned with H'H, as are balanced incomplete block designs. This latter observation led to an investigation of the second class. We showed, by example, that neither one of these classes is uniformly better than the other.

The efficiency-consistency of Kronecker product designs leads one to consider Kronecker products of other highly efficient designs such as group divisible designs when balanced incomplete block designs do not exist. Table 1 shows that this is a reasonable strategy.

Table 1. Efficiencies of GD-Kronecker product designs

m_1	n_1	k_1	b_1	λ_{11}	λ_{12}	m_2	n_2	k_2	b_2	λ_{21}	λ_{22}	e_d
3	2	3	4	0	1	3	2	3	4	0	1	.985
3	2	4	3	2	1	3	2	4	3	2	1	.985
3	2	4	3	2	1	3	2	3	4	0	1	.985
2	4	4	12	2	3	3	2	4	3	2	1	.989
2	4	4	12	2	3	2	4	4	12	2	3	.993
4	2	3	8	0	1	3	2	3	4	0	1	.989
4	3	4	9	0	1	3	2	3	4	0	1	.990
4	3	4	9	0	1	2	4	4	12	2	3	.993
4	3	4	9	0	1	4	3	4	9	0	1	.999
5	4	5	16	0	1	2	4	4	12	2	3	.993
6	5	6	25	0	1	3	2	3	4	0	1	.995

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