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Optimal block designs revisited: An approximate theory detour

Friedrich Pukelsheim[a,*], Bikas Kumar Sinha[b]

[a] *Universität Augsburg, 86135 Augsburg, Germany*
[b] *Indian Statistical Institute, Calcutta 700 035, India*

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Abstract

The paper reviews and merges optimality properties of block designs in the approximate theory and in the exact theory. Emphasis is on balanced incomplete block designs, although more general block designs are also treated. A correct version of an erroneous statement in Pukelsheim (1993) is given.

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1. Introduction

The paper is an attempt to understand and extend some known results on optimal block designs from the viewpoint of the approximate optimality theory, as well as the exact optimality theory. An in-depth discussion of the exact theory is given by Shah and Sinha (1989), while the approximate theory is presented in Pukelsheim (1993).

Use of the approximate optimality theory for regression designs is an established fact. To the contrary, in exact (combinatorial) designs it appears to be more natural to employ discrete optimization techniques. However, the juxtaposition of the two approaches is much less pronounced than would seem at first glance, and Section 14.9 of Pukelsheim (1993) makes an attempt towards deriving optimality properties of block designs within the approximate theory.

This note has the primary objective to have a fresh look into the technical proof of optimality of balanced incomplete block designs (BIBDs) and related block designs from the two different viewpoints, and develop from this a wider appreciation for such optimality properties. We strengthen some known optimality statements on BIBDs, and discuss their domain of validity. We also correct an erroneous statement in Section 14.9 of Pukelsheim (1993).

* Corresponding author.

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2. Optimality of BIBDs in the approximate theory

The classical proof of universal optimality of a BIBD rests on two properties. Firstly, the associated contrast information matrix (also known as C-matrix) is completely symmetric, that is, the on-diagonal elements are the same and the off-diagonal elements are the same. Secondly, the contrast information matrix has maximum trace among the competing C-matrices. The proof uses the fact that the frequencies n_{ij} for observing treatment i in block j trivially satisfy

$$n_{ij}^2 \geqslant n_{ij}. \tag{1}$$

In the approximate theory, the frequencies n_{ij} are replaced by weights w_{ij} that are nonnegative and add to one. However, inequality (1) no longer holds true with arbitrary $w_{ij} \in (0, 1)$ replacing n_{ij}. This is the first obstacle towards a direct derivation of optimality properties of BIBDs using the approximate theory.

In an attempt to circumvent this difficulty, Pukelsheim (1993, Section 14.9) makes the *total support assumption* to restrict the class of competing designs to those which have the same or a smaller support than the given BIBD.

The technical effect is the following. Every BIBD is binary, that is its frequencies n_{ij} are either 0 or 1. Let w_{ij} be the weights of a competing design that satisfies the total support assumption, that is

$$n_{ij} = 0 \;\Rightarrow\; w_{ij} = 0. \tag{2}$$

Then the given BIBD and the competing design are tied together through the relation $w_{ij} = n_{ij} w_{ij}$. This seems to lead the rescue operation in the approximate theory.

We begin by relaxing the total support assumption (2) while dealing with the approximate theory. Instead we impose the *block support assumption* that *no more than k entries in any block are positive.* Within this class, a given BIBD with parameters b, v, r, k, λ remains universally optimal. The concept of *universal optimality* is discussed in detail by Shah and Sinha (1989, Ch. 2), while Pukelsheim (1993, Section 14.9) subsumes it under the more general notion of *Kiefer optimality*.

Theorem 1. *Let $N = ((n_{ij}))$ be the incidence matrix of a BIBD for v varieties in b blocks, with replication number r, block size k, and concurrence number λ, for a total of $n = bk = vr$ observations. Let $\mathscr{W}(k)$ be the class of those $v \times B$ weight matrices W that have an arbitrary number B of columns each of which has at most k positive entries. Then the approximate version of the BIBD, N/n, lies in the set $\mathscr{W}(k)$, and is universally optimal for inference on the varietal contrasts within the class $\mathscr{W}(k)$.*

Proof. First observe that the approximate BIBD allocates uniform weight $1/n$ over the nonvanishing entries in N. For a competing design with B blocks, let W be the weight matrix of order $v \times B$. The block support assumption means that the number t_j of positive entries in column j of W satisfies $t_j \leqslant k$, for $j = 1, \ldots, B$.

The trace of the C-matrix that belongs to W is given by $1 - \sum_{j=1}^{B} \sum_i w_{ij}^2 / w_{.j}$, where $w_{.j}$ is the sum of the entries in column j of W. For each j, the Cauchy inequality yields $w_{.j}^2 \leqslant t_j \sum_i w_{ij}^2$. This is used to bound the trace of the C-matrix from above,

$$1 - \sum_{j=1}^{B} \frac{\sum_i w_{ij}^2}{w_{.j}} \leqslant 1 - \sum_{j=1}^{B} \frac{w_{.j}}{t_j} \leqslant 1 - \frac{1}{k}. \tag{3}$$

The second inequality in (3) uses the block support assumption $t_j \leqslant k$. □

We find it remarkable that, in the presence of the block support assumption, no restriction is placed on the number of blocks B. The block support assumption itself cannot be entirely omitted as, otherwise, a design with uniform weight $1/(Bv)$ will turn out to be better than a BIBD whenever $B > b$.

Equality throughout (3) forces each block to have k weights equal to $w_{.j}/k$, and $v-k$ weights equal to zero. This is not enough to characterize BIBDs, and other designs may perform just as well. For instance, the BIBD

$$N=\begin{pmatrix}1&1&0&1&1&0\\1&0&1&1&0&1\\0&1&1&0&1&1\end{pmatrix}$$

leads to the approximate design $N/12 \in \mathscr{W}(2)$. It has the same C-matrix as the competing approximate design

$$W=\frac{1}{18}\begin{pmatrix}2&2&0&1&1&0\\2&0&2&1&0&1\\0&2&2&0&1&1\end{pmatrix}\in \mathscr{W}(2),$$

which does not arise from a BIBD! The approximate design W is interpreted as taking 18 observations on 3 varieties in 6 blocks, where block 1 (= column 1) contains 2 observations on each treatment 1 and 2, block 2 contains 2 observations on treatments 1 and 3, etc.

3. Optimality of BIBDs in the exact theory

The exact version of Theorem 1 says that a BIBD is universally optimal within the class of those block designs for which each block is at most of size k.

In the exact theory the block support assumption can be dispensed with provided the number of blocks B of the competing designs is greater than or equal to the number of blocks b of the given BIBD. This intuitively plausible relation means that more blocks are detrimental to the information that is available on the treatments. The precise result is contained in the following theorem.

Theorem 2. *Let $N=((n_{ij}))$ be the incidence matrix of a BIBD for v varieties in b blocks, with replication number r, block size k, and concurrence number λ, for a total of $n=bk=vr$ observations. Let $\mathscr{D}(b)$ be the class of those exact designs for n observations on v varieties that have $B \geqslant b$ blocks (and each block has at least one positive entry).*

Then the BIBD N lies in the set $\mathscr{D}(b)$, and is universally optimal for inference on the varietal contrasts within the class $\mathscr{D}(b)$.

Proof. The usual argument based on the trivial inequality (1) immediately yields the upper bound $1-B/n$ for the trace of the C-matrix of a (standardized) competing design. This is further dominated by the corresponding quantity $1-b/n$ for the (standardized) BIBD. □

Theorem 2 does not permit a statement on uniqueness. All we can say is that a block design which is universally optimal in $\mathscr{D}(b)$ must be binary, and must be supported on exactly b blocks. But it need not necessarily be a BIBD! A counterexample is design N_4 of Exhibit 14.2 in Pukelsheim (1993, p. 370).

A more general family of counterexamples occurs with the BIBDs in the Yates' orthogonal series of Section 5.9 in Raghavarao (1971), having the parameters

$$v=s^2,\quad b=s^2+s,\quad r=s+1,\quad k=s,\quad \lambda=1.$$

Note that $n = bk = s(s^2 + s) = sv + s^2$. Therefore, as a competitor design, we may have one with s complete blocks and an additional set of s^2 blocks each of size 1 with entirely arbitrary composition. This provides a completely symmetric C-matrix with trace $1 - b/n$. Hence all such designs are equivalent to the BIBD!

4. Nonoptimality of BIBDs in the exact theory

We now express more serious concern when the number of blocks B is allowed to be strictly less than the number of blocks b in the candidate BIBD. Optimality of the BIBD fails immediately when B is as small as possible, $B = 1$. For example, in Exhibit 14.2 of Pukelsheim (1993, p. 370) the one-block design N_1 is better than the BIBD N_2.

But even if B is just somewhat smaller than b, at best $B = b - 1$, we can no longer claim optimality of the BIBD. This disappointing fact is brought out by the following example, with parameter values

$$v = 4, \quad b = 12, \quad r = 6, \quad k = 2, \quad \lambda = 2.$$

It is readily seen that two copies of the unreduced BIBD composed of four treatments taken two at a time provides a BIBD with parameters as given above. We now opt for $B = 11$. Following Cheng (1979) the blocks of our competing design are taken to be

$$(1,2)\,(1,3)\,(1,4)\,(2,3)\,(2,4)\,(3,4)\,(1,3)\,(1,4)\,(2,3)\,(2,4)\,(1,2,3,4).$$

It is easy to verify that the C-matrix of the competitor design has positive eigenvalues 4, 4, 5, while the C-matrix of the BIBD has eigenvalues 4, 4, 4. Hence the competitor uniformly dominates the BIBD!

It must be noted that in the case of a binary design for n observations in B blocks, the trace of the C-matrix is given by $n - B$. This is larger than the corresponding quantity $n - b$ of the BIBD whenever B is smaller than b. The example above further shows that the competing design has uniform dominance over the BIBD even though its C-matrix is not completely symmetric.

It is also possible to construct examples of binary designs with B smaller than b that do possess a completely symmetric C-matrix. Interesting examples are built from component designs which have unequal block sizes. The C-matrix of such components is far from being completely symmetric. One such example is the following.

Consider the design d_1 with $n = 1530$ observations spread over 51 copies of a BIBD with parameters

$$v = 6, \quad b = 15, \quad r = 5, \quad k = 2, \quad \lambda = 1.$$

The competitor design d_2 consists of 10 copies of the component design d_3 given by 2 copies of the subcomponent design d_{31}, 6 copies of the subcomponent design d_{32}, and 3 copies of the subcomponent design d_{33}. The subcomponent designs are defined through their blocks:

$$\begin{aligned}
d_{31}:\ & (1,4)\,(1,5)\,(1,6)\\
& (2,4)\,(2,5)\,(2,6)\\
& (3,4)\,(3,5)\,(3,6),\\
d_{32}:\ & (4,4)\,(5,5)\,(6,6),\\
d_{33}:\ & (1,2,4)\,(1,3,4)\,(2,3,4)\\
& (1,2,5)\,(1,3,5)\,(2,3,5)\\
& (1,2,6)\,(1,3,6)\,(2,3,6).
\end{aligned}$$

The C-matrices of the designs d_1 and d_2 are of the form $\rho_i K_6$, where $K_6 = I_6 - 1_6 1_6'/6$. The coefficients are found to be $\rho_1 = 153$ and $\rho_2 = 180$, respectively, so that the design d_1 is dominated by d_2 outright!

5. Nonoptimality of BIBDs in the approximate theory

In our final analysis of optimality of the BIBDs, we turn to the approximate theory to reexamine some of the results established in the exact theory. Theorem 2 states that, for $B \geqslant b$, the BIBDs are optimal in the class of *all* competing designs with B blocks, irrespective of the block compositions. In the exact theory, it is clear that when we speak of the presence of B blocks, we then mean that each block contains at least one observation. In the approximate theory, there are at least three distinct ways of expressing this phenomenon.

Firstly, we may demand that each column of a $v \times B$ weight matrix W should have at least one positive entry. This immediately negates the optimality of the BIBD since the design with uniform weight $1/(Bv)$ is better.

Secondly, we may demand that every entry w_{ij} must satisfy the requirement that nw_{ij} is a nonnegative integer. This retains the unique optimality property of the BIBDs, for the evident reason that it is just a disguised form of embedding the exact theory into the approximate theory.

Thirdly, we may demand for every column j of W that $nw_{\max,j} \geqslant 1$, where $w_{\max,j}$ stands for the largest weight among $w_{1j}, \ldots, w_{vj}$. This ensures that each of the B blocks of W contains at least one observation. Even with this understanding, it turns out that there are competing designs with larger traces unless B is really large. We examined this situation for $k = 2$ and $k = 3$, only to find that we need $B \geqslant n - 2$ at least. This comes as a highly discouraging fact.

What all this amounts to, in our eyes, is that the exact optimality theory and the approximate optimality theory for block designs are not entirely identical. Both approaches contribute to our understanding of optimal block designs, but in a complementary fashion. The approximate theory emphasizes the optimality properties which are shared between block designs and regression designs, on the grounds that both are instances of the general design problem. As soon as the inherent discreteness of block designs enters into the discussion, the approximate theory comes to an end and the exact theory takes over.

6. A counterexample

Two of the five parameters that are usually quoted with a BIBD are redundant in that they can be expressed as functions of the other three. For example, the common treatment replication number and the common block size can be expressed as $r = n/v$ and $k = n/b$. Hence we can speak of a BIBD for n observations on v varieties in b blocks. These three parameters are also sufficient to formulate the optimality result in our Theorem 1: There are $v - 1$ varietal contrasts, and the class of competing designs in $\mathscr{W}(n/b)$.

In contrast, the optimality statement in Pukelsheim (1993, p. 368) relates optimality of a given BIBD to a set of competing block designs that is restricted by the support of the given BIBD. On p. 369 an attempt is made to extend optimality from a class of designs restricted by the location of their support points, to a larger class for which the characterization does not require more knowledge than is supplied by the three parameters n, v, b.

The following counterexample shows why that optimality extension is in error. Consider the following two BIBDs N and $\tilde{N}$ for 6 observations on 3 varieties in 3 blocks,

$$N = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \qquad \tilde{N} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The union of the support sets of N and $\tilde{N}$ is the full set of *all* variety block combinations. The statement in the first printing of Pukelsheim (1993, p. 369) then asserts optimality of the given BIBDs among *all* block designs, and this is apparently false. The appropriate optimality extension is Theorem 1 of the present paper, as included in the second and subsequent printings of Pukelsheim (1993).

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