OPTIMAL INCOMPLETE BLOCK DESIGNS

FOR COMPARING TREATMENTS WITH A CONTROL

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ABSTRACT

The problem of finding optimal incomplete block designs for comparing \( p \) test treatments with a control is studied. B.I.B. designs are found to be D-optimal. A- and E-optimal designs are also obtained. For a large class of functions \( \phi \), conditions for a design to be \( \phi \)-optimal are found. Most of the optimal designs are certain types of B.T.I.B. designs (introduced by Bechhofer and Tamhane (1981)) which are binary in test treatments.

Keywords and phrases: Incomplete block designs, BTIB designs, BIB designs, binary designs, comparing \( p \) treatments to a control, \( \phi \)-optimality, D-optimality, A-optimality, E-optimality.

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1. Introduction

Consider an experimental situation where it is desired to compare \( p \geq 2 \) test treatments to a control treatment. Let the \( p + 1 \) treatments be indexed \( 0, 1, \ldots, p \) with \( 0 \) denoting the control treatment and \( 1, 2, \ldots, p \) denoting the test treatments. It is desired to compare simultaneously the \( p \) test treatments to the control. For improving the precision of the comparisons the experimental units are to be blocked in \( b \) blocks each of size \( k, 2 \leq k \leq p \). We are then in an incomplete block design setting.

Let \( Y_{ijh} \) denote the observation on treatment \( i(0 \leq i \leq p) \) in block \( j(1 \leq j \leq b) \) in plot \( h(1 \leq h \leq k) \). We assume the usual additive linear model without interactions, namely

\[
Y_{ijh} = \mu + \alpha_i + \beta_j + \epsilon_{ijh},
\]

the \( \epsilon_{ijh} \) are assumed to be uncorrelated random variables with mean 0 and common variance \( \sigma^2 \). The \( p \) control-treatment contrasts \( \alpha_0 - \alpha_i \) are to be estimated by their BLUEs \( \hat{\alpha}_0 - \hat{\alpha}_i \) (\( 1 \leq i \leq p \)). It is desired to choose an experimental design (an allocation of treatments to blocks) which will yield the best, in some sense, set of estimates among all possible designs.

For given values of \( b, k, \) and \( p \) let \( C(b, k, p) \) denote the class of all possible incomplete block designs with \( b \) blocks, each of size \( k(p \geq k \geq 2) \), \( p \) test treatments indexed \( 1, \ldots, p \), and a control treatment indexed \( 0 \).

For a design \( d \in C(b, k, p) \) let \( r_{ij}(d) \) denote the number of replications of treatment \( i(0 \leq i \leq p) \) in block \( j(1 \leq j \leq b) \). Also let \( r_i(d) = \sum_{j=1}^{b} r_{ij}(d) \) and \( \lambda_{i\ell}(d) = \sum_{j=1}^{b} r_{ij}(d)r_{\ell j}(d) \) (\( 0 \leq i \neq \ell \leq p \)). Notice \( r_i(d) \) represents the number of replications of treatments in the entire design \( d \) and \( \lambda_{i\ell}(d) \) represents the number of times treatments \( i \) and \( \ell \) are paired together in a block summed over all blocks.
For \( d \in C(b,k,p) \), let \( M(d) \) denote the information matrix corresponding to estimating all \( \alpha_0 - \alpha_i, 1 \leq i \leq p \), (as in Bechhofer and Tamhane (1981)). \( M(d) \) is a nonnegative definite \( p \times p \) matrix and is nonsingular if and only if all the \( \alpha_0 - \alpha_i \) are estimable, in which case it is proportional to the inverse of the covariance matrix of \( \hat{\alpha}_0 - \hat{\alpha}_i, 1 \leq i \leq p \).

We now make our goal of finding a design \( d \in C(b,k,p) \) which gives us the best, in some sense, set of BLUEs \( \hat{\alpha}_0 - \hat{\alpha}_i, 1 \leq i \leq p \) more explicit. Following the work of Kiefer (see for example Kiefer (1958, 1959, 1971, and 1974)) we seek a \( d \in C(b,k,p) \) which minimizes \( \phi(M(d)) \) for some function \( \phi \) over \( C(b,k,p) \). Such a design will be called \( \phi \)-optimal. Restricting to non-singular designs, some common examples of \( \phi \) are \( \phi_0(M(d)) = \det M^{-1}(d) \) (so called D-optimality), \( \phi_1(M(d)) = \text{tr} M^{-1}(d) \) (so called A-optimality), and \( \phi_\infty(M(d)) = \text{maximum eigenvalue of } M(d) \) (so called E-optimality). In the present context of control-treatment comparisons, A-optimality has an appealing statistical interpretation, viz. it minimizes \( \sum_{i=1}^{p} \text{var}(\hat{\alpha}_0 - \hat{\alpha}_i) \) over all designs. We are, however, yet to realize natural statistical interpretations for the other criteria.

Traditionally, Kiefer and other researchers were interested in an orthonormal basis of treatment contrasts. In other words, the aim was to determine good designs for estimating \( P\hat{\alpha} \) where \( \hat{\alpha} \) is the vector of all the \( p+1 \) treatment effects and \( P \) is a \( p \times p+1 \) matrix of zero row sums and orthonormal rows. Nothing much seems to be known for the situation when the contrasts are not mutually orthogonal. In this paper we look at one such situation - that of control-treatment comparison.

Let \( \psi_i(d), 1 \leq i \leq p \), be the positive eigenvalues of the well known "C-matrix" of normal equations for \( \hat{\alpha} \), for a design \( d \) in \( p+1 \) treatments in \( b \) blocks of \( k \) plots each. Let \( P\hat{\alpha} \) be any vector of \( p \) independent
treatment contrasts, and \( V(P_d^\top) \) be the covariance matrix of the BLUE's of \( P_d \). Then it can be shown that

\[
\text{det} V(P_d^\top) = (\text{det}(PP'))(\nu_1(d)\ldots\nu_p(d))^{-1}.
\]

This can be established by starting from a spectral decomposition of the C-matrix for the design d, or by proving a result like equation (A.2) of Bechhofer and Tamhane (1981). Since a B.I.B. design, if it exists, is D-optimal in the traditional sense of estimating orthonormal contrasts, we have the following theorem.

**Theorem 1.1** A B.I.B. design, if it exists, is D-optimal for estimating any set of p independent treatment contrasts.

It has come to our notice that this result has been known for some time by Hedayat (1974) and Kiefer (the result follows easily from section 3 of Kiefer (1958)). Observe that the D-optimality criterion ignores the particular interests of the experimenter expressed through the matrix \( P \).

From the work of Kiefer and others on optimal incomplete block designs for estimating an orthonormal basis of treatment contrasts, it is known that the B.I.B. design is optimal, not only according to the D-criterion, but under a very large class of optimality criteria as well (see Kiefer (1958, 1959, 1971, 1974 and 1975)). Such results might lead us to expect that in our setting an optimal design \( d \) in \( C(b,k,p) \) would be symmetric (in some sense) and binary in the test treatments \( 1,\ldots,p \) (but not in the control). Since the control plays a special role in our setting we might also expect that the number of replications of the control (more specifically the \( r_{0j}(d) \)) will be an important factor in determining what design \( d \) is optimal. These expectations are indeed found to be the case as will be seen in the results of section 2.
The proper sense of symmetry in a design \( \mathbf{d} \in C(b,k,p) \) turns out to be that all \( \lambda_{i\ell}(\mathbf{d}) \) are equal for \( 1 \leq i \neq \ell \leq p \) and all \( \lambda_{0\ell}(\mathbf{d}) \) for \( 1 \leq \ell \leq p \) are equal (but not necessarily to the \( \lambda_{i\ell}(\mathbf{d}) \) for \( 1 \leq \ell \leq p \)). Such designs are called balanced treatment incomplete block designs (abbreviated BTIBs) and were first introduced in Bechhofer and Tamhane (1981) in connection with making joint confidence statements about the contrasts \( \alpha_0 - \alpha_i \), \( 1 \leq i \leq p \). The interested reader is referred to this paper for more information on BTIB designs. We remark that if a design \( \mathbf{d} \in C(b,k,p) \) is a BTIB design its information matrix \( M(\mathbf{d}) \) is completely symmetric (i.e. all off diagonal elements equal and all diagonal elements equal). Bechhofer and Tamhane (1981) also have a review on available literature for designs for control-treatment comparisons.

Section 2 of this paper contains results about what designs are \( \Phi \)-optimal for a fairly broad class of functions \( \Phi \). As an important application we discuss A-optimal designs.

The class of functions considered in section 2 does not include E-optimality. This is treated in section 3, which also includes a result showing that an A-optimal design is optimal according to another statistically interesting criterion. Section 4 contains some concluding remarks.

2. A-Optimal Designs

We begin this section with a series of lemmas culminating in a general theorem from which A-optimal designs may be obtained as a special case.

Suppose \( \mathbf{d} \in C(b,k,p) \) is arbitrary. Let \( \mathcal{I} \) be the set of all \( p! \) permutations of the test treatments \( 1, \ldots, p \). Let \( \sigma \mathbf{d}, \sigma \in \mathcal{I} \), be the design resulting from \( \mathbf{d} \) by the permutation \( \sigma \) of the treatments in \( \mathbf{d} \). We define

\[
M(\mathbf{d}) = \sum_{\sigma \in \mathcal{I}} \frac{M(\sigma \mathbf{d})}{p!} = \sum_{\pi \in \Pi} \frac{\pi' M(\mathbf{d}) \pi}{p!}
\]

where \( \Pi \) is the set of all \( p \times p \) permutation matrices. It is easily seen
that when $\bar{M}(d)$ is the information matrix of some design then this design is a B.T.I.B. design (Bechhofer and Tamhane (1981)).

Lemma 2.1. If $d \in C(b,k,p)$ then $\bar{M}(d)$ has eigenvalues $\nu_1(d)$, $\nu_2(d) = \ldots = \nu_p(d)$ with

$$\nu_1(d) = \left\{ \sum_{i=1}^{p} \frac{\lambda_{0i}(d)}{k}/p = \frac{r_0(d)}{k} - \sum_{j=1}^{b} \frac{r_{0j}(d)}{k}/p \right\}$$

$$\nu_2(d) = \left\{ \sum_{i=1}^{p} \frac{r_i(d)}{k} - \sum_{j=1}^{b} \frac{r_{ij}(d)/(k-(r_0(d)-\sum_{j=1}^{b} \frac{r_{0j}(d)}{p})/(p-1))}{k} \right\}$$

In addition if $d$ is binary in test treatments

$$\nu_2(d) = \{b(k-1)-((k-1)/k)r_0(d)-(r_0(d)-\sum_{j=1}^{b} \frac{r_{0j}(d)/p}{p})/(p-1)\}$$

pf. From the appendix of Bechhofer and Tamhane (1981), the entries of $M(d)$ are

$$m_{i_1i_2} = \begin{cases} r_i(d) - \sum_{j=1}^{b} \frac{r_{ij}(d)/k}{k} & (i_1=i_2) \\ -\frac{\lambda_{ij}(d)/k}{k} & (i_1 \neq i_2) \end{cases}$$

and the sum of the entries in the $i$-th row (or $i$-th column) is $\lambda_{0i}/k$.

Thus is it straightforward to check that

$$\overline{M}(d) = \left( \sum_{i=1}^{p} \frac{r_i(d)}{k} - \sum_{i=1}^{p} \sum_{j=1}^{b} \frac{r_{ij}(d)/k}{k} + \sum_{1 \leq i_1 \neq i_2 \leq p} \frac{\lambda_{i_1i_2}/(k(p-1))}{p} \right) \overline{I}_p$$

$$- \left( \sum_{1 \leq i_1 \neq i_2 \leq p} \frac{\lambda_{i_1i_2}}{kp(p-1)} \right) J_{p,p}$$

where $I_p$ is the $p \times p$ identity matrix and $J_{p,p}$ is the $p \times p$ matrix all of whose entries are +1. The first part of the lemma now follows from the well known fact that $aI_p + bJ_{p,p}$ has eigenvalues $a$ with multiplicity $p-1$ and $a + bp$ with multiplicity 1. The second part involves essentially straightforward computations only.
Lemma 2.2. Suppose $\phi$ is a convex real-valued possibly infinite function on the set of all $p \times p$ non-negative definite matrices and $\phi$ is invariant under permutations, i.e. if $\pi$ is a permutation matrix, $\phi(\pi'M\pi) = \phi(M)$. Then for $d \in C(b,k,p)$, $\phi(\overline{M}(d)) \leq \phi(M(d))$.

pf. $\phi(M(d)) = \sum_{\sigma \in \mathcal{S}} \phi(M(\sigma d))/p!$ since $\phi$ is permutation invariant. Thus by convexity $\phi(M(d)) \geq \phi(\sum_{\sigma \in \mathcal{S}} M(\sigma d)/p!) = \phi(\overline{M}(d))$.

Lemma 2.3. Suppose $\phi$ is some real-valued possibly infinite function on the set of all non-negative definite $p \times p$ matrices with the property that if $M$ and $N$ are non-negative definite $p \times p$ matrices with eigenvalues $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_p$ and $\nu_1 \leq \nu_2 \leq \ldots \leq \nu_p$ respectively which satisfy $\mu_i \geq \nu_i$ for $i = 1, \ldots, p$ then $\phi(M) \leq \phi(N)$.

Let $d \in C(b,k,p)$ be a design which is not binary in test treatments. Then there exists $d^* \in C(b,k,p)$ which is binary in test treatments with $r_0(d^*) = r_0(d)$ and which satisfies $\phi(\overline{M}(d^*)) \leq \phi(\overline{M}(d))$.

pf. In each block of $M(d)$ replace any duplicates of test treatments by test treatments not in the block so that each block is binary in test treatments (this is possible since $k \leq p$). Call the resulting design $d^*$. Notice $d^*$ is binary in test treatments, has $r_{0j}(d^*) = r_{0j}(d)$ for all $1 \leq j \leq b$, and has $\sum_{i=1}^{p} r_{ij}(d^*) = \sum_{i=1}^{p} r_{ij}(d)$. As a result it is easy to see $\sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d^*) \leq \sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d)$.

From lemma 2.1 it then follows that the eigenvalues of $\overline{M}(d)$ and $\overline{M}(d^*)$ satisfy $\nu_1(d) = \nu_1(d^*)$ and $\nu_2(d) = \ldots = \nu_p(d) \leq \nu_2(d^*) = \ldots = \nu_p(d^*)$. Hence by the property of $\phi$ given in the statement of the lemma, $\phi(\overline{M}(d^*)) \leq \phi(\overline{M}(d))$. 
Lemma 2.4. Among all non-negative integers $r_{01}, r_{02}, \ldots, r_{0b}$ satisfying \[ \sum_{j=1}^{b} r_{0j} = r, \] where $r$ is a fixed constant, the value of \[ \sum_{j=1}^{b} r_{0j}^2 \] is minimized by choosing $r - b[r/b]$ of the $r_{0j}$ to have value $[r/b] + 1$ and the remaining $b(1+[r/b]) - r$ of the $r_{0j}$ to have value $[r/b]$. Here $[\cdot]$ denotes the greatest integer function.

pf. This is lemma 2.3 of Cheng and Wu (1980).

Lemma 2.5. Suppose $\phi$ is as in lemma 2.3. Suppose $d \in C(b,k,p)$ is binary in test treatments and has $r_0(d) > bk/2$. Then there exists $d^* \in C(b,k,p)$ which is binary in test treatments, has $r_0(d^*) < bk/2$, and satisfies $\phi(\overline{M}(d^*)) \leq \phi(\overline{M}(d))$.

pf. Take $d^*$ to be the design where in each block of $d$ we replace all test treatments by the control and all of the original replications of the control by differing test treatments not originally in the block. Notice

\begin{equation}
(2.3) \quad r_0(d^*) = \sum_{j=1}^{b} r_{0j}(d^*) = \sum_{j=1}^{b} (k-r_{0j}(d)) = bk - r_0(d) < bk/2 < r_0(d)
\end{equation}

\begin{equation}
(2.4) \quad r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k = r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k.
\end{equation}

From (2.4) it follows that if $\mu_1(d), \mu_2(d) = \ldots = \mu_p(d)$ and $\mu_1(d^*)$, $\mu_2(d^*) = \ldots = \mu_p(d^*)$ are the eigenvalues of $\overline{M}(d)$ and $\overline{M}(d^*)$, respectively, as given in lemma 2.1, then $\mu_1(d) = \mu_1(d^*)$. Also from (2.3), (2.4), and lemma 2.1, $\mu_2(d) < \mu_2(d^*)$. By the property of $\phi$ given in the lemma it follows that $\phi(\overline{M}(d^*)) \leq \phi(\overline{M}(d))$.

Theorem 2.1. Suppose $\phi$ is a real-valued possibly infinite function on the set of all $p \times p$ non-negative definite matrices satisfying
\[ \phi(M) = \sum_{i=1}^{p} f(\mu_i) \]

where \( \mu_1 \leq \mu_2 \leq \ldots \leq \mu_p \) are the eigenvalues of \( M \), \( f \) is a real valued possibly infinite function on the set of all non-negative numbers which is continuous on the set of all positive numbers, has \( f' < 0 \) and \( f'' > 0 \) (here primes denote differentiation). Suppose there is a \( \delta \in C(b,k,p) \) such that \( M(\delta) \) is completely symmetric and

(i) \( \delta \) is binary in test treatments

(ii) \( r_0(\delta) \) is the value of the integer \( r, 0 \leq r \leq \lfloor bk/2 \rfloor \), which minimizes

\[
(2.5) \quad g(r;b,k,p) = f((r-h(r;b)/k)/p) \\
+ (p-1)f((b(k-1)-((k-1)/k)r-(r-h(r;b)/k)/p)/(p-1))
\]

where

\[
(2.6) \quad h(r;b) = (b(1+[r/b])-r)[r/b]^2 + (r-b[r/b])([r/b]+1)^2
\]

(iii) the \( r_{0j}(\delta) \) have value either \( \lfloor r_0(\delta)/b \rfloor \) or \( \lceil r_0(\delta)/b \rceil + 1 \).

Then \( \delta \) is \( \phi \)-optimal over \( C(b,k,p) \).

pf. First we notice \( \phi \) and \( f \) have the following properties

(a) \( \phi \) is convex and orthogonal invariant (i.e. if \( \pi \) is an orthogonal matrix then \( \phi(\pi'M\pi) = \phi(M) \))

(b) \( \sum_{i=1}^{p} f(\mu_i) \leq \sum_{i=1}^{p} f(\nu_i) \) if \( \mu_i \geq \nu_i \) for all \( 1 \leq i \leq p \).

(c) if \( \mu_1 \leq \mu_2 = \ldots = \mu_p, \nu_1 \leq \nu_2 = \ldots = \nu_p \), \( \mu_1 \geq \nu_1 \), and

\[
\sum_{i=1}^{p} \mu_i = \sum_{i=1}^{p} \nu_i \text{ then } \sum_{i=1}^{p} f(\mu_i) \leq \sum_{i=1}^{p} f(\nu_i).
\]

Property (a) follows from the fact that \( f'' > 0 \). Property (b) follows from the fact that \( f' < 0 \). Property (c) follows from the fact that \( \phi \) regarded as a function of \( (\mu_1, \ldots, \mu_p)' \) is Schur convex.
Now suppose $\delta$ is as given in the theorem. Let $d \in C(b,k,p)$ be any design which is binary in the test treatments. By (a) and lemma 2.2, $\phi(\bar{M}(d)) \leq \phi(M(d))$. If $r_0(d) > bk/2$ by lemma 2.5 there exists $d^* \in C(b,k,p)$ with $r_0(d^*) < bk/2$ and $\phi(\bar{M}(d^*)) \leq \phi(\bar{M}(d))$. Replace $d$ by $d^*$. If $r_0(d) \leq bk/2$ let $d^* = d$. Notice by lemma 2.1 $\bar{M}(d^*)$ has eigenvalues

$$
\mu_1(d^*) = (r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k)/p
$$

$$
\mu_2(d^*) = \ldots = \mu_p(d^*)
$$

$$
= (b(k-1)-((k-1)/k)r_0(d^*)-(r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k)/p)/((p-1)).
$$

Using the facts $k \geq 2$, $r_0(d^*) \leq bk/2$, and some calculus, one can prove that,

$$
\mu_2(d^*) \geq bk/4p
$$

$$
= \max(r_0 - \sum_{j=1}^{b} r_{0j}^2/k)/p
$$

$$
\geq \mu_1(d^*)
$$

where the maximum is over all real numbers $r_0, r_{01}, \ldots, r_{0j}$ such that $r_0 \geq 0$, $r_{0j} \geq 0$, $1 \leq j \leq b$, and $\sum_{j=1}^{b} r_{0j} = r_0 \leq bk/2$. Thus the eigenvalues $\mu_1(d^*), \mu_2(d^*), \ldots, \mu_p(d^*)$ of $\bar{M}(d^*)$ satisfy $\mu_1(d^*) \leq \mu_2(d^*) = \ldots = \mu_p(d^*)$.

Next notice

(2.7) $\phi(\bar{M}(d^*))$

$$
= f(\mu_1(d^*)) + (p-1)f(\mu_2(d^*)) = f([r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k]/p)
$$

$$
+ (p-1)f([b(k-1)-((k-1)/k)r_0(d^*)-(r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k)/p]/(p-1)).
$$
For a fixed value of \( r_0(d^*) \leq bk/2 \) we have 
\[
\nu_1(d^*) + (p-1)\nu_2(d^*) = (k-1)(b-r_0(d^*)/k) = \text{constant and the largest possible value of } \nu_1(d^*)
\]
\[
= (r_0(d^*) - \frac{1}{p} \sum_{j=1}^{b} r_{0j}^2(d^*)/k) \text{ occurs when } b(1+[r_0(d^*)/b] - r_0(d^*) \text{ of the }
\]
\[
r_{0j}(d^*) \text{ are } [r_0(d^*)/b] \text{ and } r_0(d^*) - b[r_0(d^*)/b] \text{ of the } r_{0j}(d^*) \text{ are }
\]
\[
[r_0(d^*)/b] + 1 \text{ by lemma 2.4. This choice of the } r_{0j}(d^*) \text{ maximizes } \nu_1(d^*)
\]
\[
\text{for fixed } r_0(d^*) \text{ and hence by property (c) of } \phi \text{ minimizes } \phi(\bar{M}(d^*)). \text{ If}
\]
\[
\text{we then select a value of } r_0(d^*) \leq bk/2 \text{ (with the optimal choice of the } \r_{0j}(d^*) \text{) which minimizes}
\]
\[
\text{the R.H.S. of (2.7) we see that this is precisely the value of } r_0(\delta) \text{ and the } r_{0j}(\delta) \text{ stated in the theorem. We thus con-}
\]
\[
\text{clude } \delta \text{ is a design minimizing } \phi(\bar{M}(d^*)) \text{ among all } d^* \text{ which are binary in}
\]
\[
\text{test treatments and have } r_0(d^*) \leq bk/2. \text{ Since } M(\delta) \text{ is completely symmetric, } M(\delta) = \bar{M}(\delta) \text{ and we see using lemma 2.2 that } \phi(M(\delta)) \leq \phi(\bar{M}(d)) \leq \phi(M(d))
\]
\[
(d \text{ is the design, binary in test treatments, we chose arbitrarily}) \text{ we con-}
\]
\[
\text{clude } \delta \text{ is } \phi\text{-optimal among all } d \text{ which are binary in test treatments.}
\]
\[
\text{Property (b) of } \phi \text{ and lemma 2.3 then give us that } \delta \text{ is } \phi\text{-optimal among all designs.}
\]

Theorem 2.1 is useful for finding optimal designs for many \( \phi \) such as \( \phi(M) = \sum_{i=1}^{p} \frac{D_{\nu_i}}{\nu_i} \text{ (D-optimality) and } \phi(M) = \sum_{i=1}^{p} \frac{1}{\nu_i} \text{ (A-optimality).} \)

It is not directly applicable to the problem of finding E-optimal designs, i.e. the design \( \delta \in C(b,k,p) \text{ which minimizes the maximum eigenvalue of } M^{-1}(\delta) \text{ (or maximizes the minimum eigenvalue of } M(\delta).) \)

As mentioned in the introduction A-optimal designs are statistically very meaningful. So we examine such designs in some detail. A design \( d \in C(b,k,p) \text{ is A-optimal if it minimizes } \text{tr } M^{-1}(d) \text{ over } C(b,k,p). \text{ In the} \)

notation of theorem 2.1 this means \( \phi(M(d)) = \text{tr } M^{-1}(d) \text{ and } f(\nu) = 1/\nu. \)

Equations (2.5) and (2.6) then become
(2.7) \[ g(r;b,k,p) = \frac{p}{r-(h(r;b)/k)} \]
\[ + \frac{(p-1)^2}{(b(k-1)-r(k-1))/k-(r-h(r;b)/k)/p} \]

with

(2.8) \[ h(r;b) = \frac{[r/b]^2(b+b[r/b]-r)}{+ (r-b[r/b])([r/b]+1)^2}. \]

The following result result is a consequence of theorem 2.1.

Theorem 2.2. Suppose R is the value of the integer \( r \), \( 0 \leq r \leq [bk/2] \), which minimizes \( g(r;b,k,p) \) as given in (2.7). Also suppose \( \delta \in C(b,k,p) \) is a B.T.I.B. design such that

(i) \( \delta \) is binary in test treatments

(ii) \( r_0(\delta) = R \)

(iii) \( r_{0j}(\delta) = [R/b] \) or \([R/b] + 1 \) for \( 1 \leq j \leq p \)

then \( \delta \) is A-optimal over \( C(b,k,p) \).

The integer \( r \) which minimizes \( g(r;b,k,p) \) can easily be found using a computer. As an example, \( r = 18 \) minimizes \( g(r;24,3,9) \) and the following B.T.I.B. design is therefore A-optimal.

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 3 & 4 & 5 \\
1 & 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 5 & 5 & 6 & 7 & 7 & 2 & 6 & 3 & 4 & 5 & 8 \\
3 & 4 & 5 & 8 & 4 & 5 & 7 & 8 & 5 & 7 & 9 & 6 & 9 & 6 & 8 & 9 & 8 & 9 & 9 & 7 & 6 & 8 & 7 & 9
\end{pmatrix}
\]

Here columns correspond to blocks and the numbers are the treatment labels.

Having determined the integer \( R \), the next step is to investigate whether a B.T.I.B. design satisfying (i)-(iii) exists or not. Writing \( q = [R/b] \) and \( a = R - bq \), an A-optimal design looks like

\[
d = \begin{pmatrix}
d(1) \\
2\end{pmatrix},
\]

where \( d(1) \) consists of \( q \) plots in each of \( b \) blocks and \( d(2) \) the rest of the \( k - q \) plots in the blocks. \( d(1) \) consists entirely of the control, while \( d(2) \) is binary in all \( p + 1 \) treatments with the control appearing \( a \) times.
The A-optimal design shown above gives an example of \( d = d_{(2)} \) since here \( q = 0 \).

If \( a = 0 \), then \( d_{(2)} \) has to be a B.I.B. design in the \( p \) test treatments. The following table gives some examples of A-optimal designs having this structure.

<table>
<thead>
<tr>
<th>b</th>
<th>k</th>
<th>b</th>
<th>q</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>14</td>
<td>4</td>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>4</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>4</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>6</td>
<td>25</td>
<td>1</td>
</tr>
</tbody>
</table>

Let us denote by \( d_q \) a design in \( C(b,k,p) \) which is a B.I.B. in the \( k - q \) plots of \( b \) blocks in the \( p \) test treatments, augmented by the control in each of the remaining \( q \) plots of \( b \) blocks. Designs of this type have been mentioned briefly by Cox (1958, p. 238); Pešek (1974) has look at \( d_1 \). Neither of them have considered these as optimal designs. The interested reader may find their efforts put in perspective in Bechhofer and Tamhane (1981). We shall now show that for many \( q \), \( d_q \) cannot be a very bad design - it is at least A - better than a B.I.B. design in all \( p + 1 \) treatments.

A B.I.B. design is a binary B.T.I.B. design with \( r_0(d) = bk/(p+1) \). Moreover, for any B.T.I.B. design, \( \text{tr} \ M(d)^{-1} = g(r_0(d);b,k,p) \). Hence we look at the sign of the function,

\[
(2.9) \quad g_1(q) = g(qb;b,k,p) - g(bk/(p+1);b,k,p)
\]

\[
= p\{r-(bq^2)/k\} + (p-1)^2/(b(k-1)-r(k-1))/k-(r-(bq^2)/k)/p\} - 2p^2/(b(k-1)) ,
\]

with \( q \) allowed to be positive integers only. If one allows \( q \) to be any
real number, then it is easy to see that the polynomial equation

\[ g_1(q) = 0 \]

has no roots in the interval \([1, (k-1)/2]\) of \(q\). Moreover \(g_1(1) < 0\) and \(g_1((k-1)/2) < 0\), but \(g_1(k/2) > 0\). Thus in particular \(g_1(q) < 0\), \(q = 1, 2, \ldots, [(k-1)/2]\). We summarize this in the following theorem.

**Theorem 2.3.** \(d_q\) is A-better than a B.I.B. design in all \(p + 1\) treatments for all \(q = 1, 2, \ldots, [(k-1)/2]\), whenever they exist.

**Remark.** Recently Constantine (1981) has also obtained some results on A-optimal designs in a subclass of all block designs.

3. E-Optimal Designs

We now determine E-optimal designs.

**Theorem 3.1.** If there exists \(\delta \in C(b, k, p)\) such that

(i) every block contains exactly \(k/2\) replications of the control, if \(k\) is even, or either \([k/2]\) or \([k/2]+1\) replications of the control if \(k\) is odd

and

(ii) \(\lambda_{01}(\delta) = \lambda_{02}(\delta) = \ldots = \lambda_{0p}(\delta)\)

then \(\delta\) is E-optimal over \(C(b, k, p)\).

**pf.** We first show that \(\lambda_{01}(\delta)/k\) is the minimum eigenvalue of \(M(\delta)\). To see this, notice that the sum of the entries in the \(i\)-th row of \(M(\delta)\) is \(\lambda_{0i}(\delta)/k\). Since \(\lambda_{0i}(\delta) = \lambda_{0i}(\delta)\) for all \(i\), all the row sums of \(M(\delta)\) are \(\lambda_{01}(\delta)/k\). It therefore follows that the \(p \times 1\) vector \((1, 1, \ldots, 1)'\) is an eigenvector of \(M(\delta)\) with eigenvalue \(\lambda_{01}(\delta)/k\).

To verify that \(\lambda_{01}(\delta)/k\) is the smallest eigenvalue of \(M(\delta)\), let \(\vec{e}\) be any eigenvector of \(M(\delta)\) other than \((1, \ldots, 1)'\). Without loss of generality we may assume the largest coordinate in absolute value of \(\vec{e}\) is +1. Suppose +1 is the \(i\)-th coordinate of \(\vec{e}\). Let \(\lambda\) denote the eigenvalue
of $M(\delta)$ corresponding to the eigenvector $\hat{e}$. Let $e_j$ denote the $j$-th coordinate of $\hat{e}$ and $m_{ij}(\delta)$ the $i,j$-th entry of $M(\delta)$. The $i$-th coordinate of $M(\delta) \hat{e}$ is

$$
\sum_{j=1}^{p} m_{ij}(\delta) e_j = e_i m_{ii}(\delta) + \sum_{j \neq 1}^{p} e_j m_{ij}(\delta) \geq m_{ii}(\delta) + \sum_{j \neq 1}^{p} m_{ij}(\delta)
$$

$$
= \sum_{j=1}^{p} m_{ij}(\delta) = \lambda_{0i}(\delta)/k = \lambda_{0i}(\delta)/k.
$$

The inequalities above follow from the fact that $e_i = \pm 1$, $|e_j| \leq 1$ for all $j$, and $m_{ij}(\delta) \leq 0$ for $i \neq j$. Since $\lambda \hat{e} = M(\delta) \hat{e}$ and the $i$-th coordinate of $\lambda \hat{e}$ is $\lambda e_i = \lambda$, we have $\lambda \geq \lambda_{0i}(\delta)/k$.

Since $\hat{e}$ was an arbitrary eigenvector, hence $\lambda$ was an arbitrary eigenvalue, we conclude $\lambda_{0i}(\delta)/k$ is the minimum eigenvalue of $M(\delta)$.

Notice

$$
\lambda_{0i}(\delta)/k = \frac{\sum_{i=1}^{p} \lambda_{0i}(\delta)/k}{p} = \frac{\sum_{j=1}^{b} r_{0j}(\delta)/k}{p}.
$$

By a proof similar to that used in lemma 2.4 one can show that among all integers $r_{01}, r_{02}, \ldots, r_{0b}$ such that $0 \leq r_{0j} \leq k$, the value of

$$
r_0 - \sum_{j=1}^{b} r_{0j}/k = (r_0 - \sum_{j=1}^{b} r_{0j})
$$

is maximized by choosing all $r_{0j} = k/2$ if $k$ is even or $r_{0j} = [k/2]$ or $[k/2] + 1$, $j = 1, \ldots, b$, if $k$ is odd. Since these are precisely the values of the $r_{0j}(\delta)$ we conclude

$$(3.1) \quad \min \text{eigenvalue of } M(\delta) = \frac{(r_0(\delta) - \sum_{j=1}^{b} r_{0j}(\delta)/k)}{p} \geq \frac{(r_0(d) - \sum_{j=1}^{b} r_{0j}(d)/k)}{p}$$

for all $d \in C(b, k, p)$. For any $d \in C(b, k, p)$
\[\min \text{eigenvalue of } M(d) = \min \hat{\mathbf{u}}^T M(d) \hat{\mathbf{u}} \quad ||\hat{\mathbf{u}}|| = 1\]

\[\leq (1, 1, \ldots, 1)^T M(d)(1, 1, \ldots, 1)/p\]

\[= \sum_{i=1}^{p} \frac{m_{ij}(d)}{p} = \sum_{i=1}^{p} \frac{\lambda_{0i}(d)}{kp}\]

\[\leq \min \text{eigenvalue of } M(\delta)\]

where we have used the facts that \[\sum_{j=1}^{p} m_{ij}(d) = \lambda_{0i}(d)/k,\]

\[\sum_{i=1}^{p} \lambda_{0i}(d)/k = r_0(d) - \frac{1}{k} \sum_{j=1}^{b} r_{0j}^2(d), \text{ and } (3.1).\]

We conclude that \(\delta\) has the largest minimum eigenvalue among all \(d \in C(b, k, p)\) and hence it follows that \(\delta\) is E-optimal over \(C(b, k, p)\). \(\square\)

The first of the following designs is E-optimal when \(b = k = p = 3\), the next two are both E-optimal when \(b = k = p = 4\) and the last is E-optimal when \(b = k = 5, p = 6\).

\[
\begin{pmatrix}
0 & 0 & 0 \\
1 & 1 & 2 \\
2 & 3 & 3
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 2 & 3 & 4
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
2 & 3 & 4 & 1 & 5
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
3 & 6 & 2 & 4 & 6
\end{pmatrix}
\]

The first two are B.T.I.B. designs; in fact the first one is A-optimal also.

Even though E-optimality is an effective way of minimizing a norm of \(M(d)^{-1}\), in the present context it does not seem to possess a very natural statistical meaning. If one favours a minimax style approach then possibly one way is to minimize the maximum variance of \((\hat{a}_0 - \hat{a}_i)\), the maximum being over \(1 \leq i \leq p\), minimum over all \(d \in C(b, k, p)\). In other words, one considers
the criterion \( \phi(M(d)) = \text{maximum diagonal entry of } M^{-1}(d) \). Since \( \phi \) is convex and permutation invariant lemma 2.2 says that \( \phi(\bar{M}(d)) \leq \phi(M(d)) \) for any \( d \in C(b,k,p) \). Furthermore, since \( \bar{M}(d) \) is completely symmetric, it is easily verified that \( \phi(\bar{M}(d)) = \text{tr } \bar{M}(d)^{-1}/p \). From these two observations it follows that if \( \delta \in C(b,k,p) \) is as in theorem 2.2 than it is \( \phi \)-optimal as well as A-optimal. This lends additional significance to the A-optimal designs.

A class of criteria that are sometimes considered in optimal design investigations (see Kiefer (1974)) are the \( \phi_q \) criteria, \( 0 < q < \infty \), where

\[
\phi_q(M(d)) = \frac{1}{p} \sum_{i=1}^{p} u_i^{-q}
\]

and \( u_1 \leq ... \leq u_p \) are the eigenvalues of \( M(d) \). D-optimality and E-optimality are limiting cases of these criteria in the sense that \( \lim_{q \to 0} (\phi_q(M(d))/p)^{1/q} = (\det M^{-1}(d))^{1/p} \) and \( \lim_{q \to \infty} (\phi_q(M(d))/p)^{1/q} = \text{max eigenvalue of } M^{-1}(d) \). In particular, \( \phi_0 \) and \( \phi_\infty \) are sometimes used to denote the D-optimality and E-optimality criteria, respectively. Also notice that \( \phi_1 \) is just the A-optimality criterion.

An examination of our above results for D-, A-, and E-optimality (or for \( \phi_0, \phi_1, \text{ and } \phi_\infty \)) indicates that the number of replications of the control in an optimal design is smallest for D-optimality, second smallest for A-optimality, and largest for E-optimality. This suggests that the number of replications of the control in a B.T.I.B. design which is \( \phi_q \)-optimal is increasing as \( q \) increases. Since \( \phi_q, 0 < q < \infty \), satisfies the conditions of theorem 2.1, it is possible (although somewhat tedious) to verify that this is indeed the case. From this it follows that if \( d \in C(b,k,p) \) is a B.T.I.B. design which is binary in test treatments with
[bk/(p+1)]<r_0(d)<b[k/2], then d is $\phi_q$-optimal for some $0 < q < \infty$.

4. Concluding Remarks

In this paper we have established optimality properties of some B.T.I.B. designs. It is hoped that this will provide added incentive for the study of these designs, particularly their construction. Observe also the dependence of optimal designs on the optimality criterion used. This is different from the usual incomplete block design setting where orthonormal treatment contrasts are of interest.

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REFERENCES


