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A-OPTIMAL BLOCK DESIGNS FOR COMPARING TEST TREATMENTS WITH A CONTROL[1]

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We consider the problem of comparing test treatments with a control in a proper block design. We give conditions on the parameters of both R-type and S-type designs that guarantee their A-optimality, and demonstrate how these conditions can be used to obtain families of A-optimal designs. We give an example for the construction of the desired S-type designs. A table with optimal R-type designs ($3 \le k \le 10$, $k \le v \le 30$) is also given.

1. Introduction. In this paper, we study the problem of comparing a set of test treatments with a control under the assumption that the experimental units can be arranged in a proper block design, a design in which all blocks have the same size. For a brief review on the available literature in this area we refer the reader to the introduction of Hedayat and Majumdar (1985). We will use the notation $D_0(v, b, k)$ for the collection of all connected block designs with b blocks of size k each, and based on v test treatments (labeled $1, \dots, v$) and a control (labeled 0). An observation Y_{ijl}, obtained by applying treatment i, $0 \le i \le v$, to an experimental unit in block j, $1 \le j \le b$, in plot l, $1 \le l \le k$, will be assumed to follow the usual additive linear model without interactions,

$$Y_{ijl} = \mu + \tau_i + \beta_j + \varepsilon_{ijl}.$$

We refer to μ as the general mean, to τ_i as the effect of treatment i and to β_j as the effect of block j. The error terms ε_{ijl} are assumed to be uncorrelated and have a common mean 0 and a common variance σ^2. The objective of the experiment is to estimate the test treatment–control contrasts $\tau_i - \tau_0$, $1 \le i \le v$. We assume that this is done by using their least squares estimates, which we will denote by $\hat{\tau}_i - \hat{\tau}_0$. These estimates will obviously be design dependent and the problem that remains is thus, for given v, b and k, to select a design $d \in D_0(v, b, k)$ that, in some sense, gives us good estimates for the contrasts of interest. In this paper, we will judge the performance of a design by the so-called A-criterion. A design $d^* \in D_0(v, b, k)$ is called A-optimal (in its class) if it minimizes

$$\sum_{i=1}^{v} \operatorname{Var}_d(\hat{\tau}_i - \hat{\tau}_0)$$

over all designs $d \in D_0(v, b, k)$. Majumdar and Notz (1983) obtained a sufficient condition for a design to be A-optimal. Utilizing this condition we will search for

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families of A-optimal designs, both R-type designs (Section 2) and S-type designs (Section 3).

2. *A*-optimal R-type designs. The following definition first appeared in Bechhofer and Tamhane (1981).

DEFINITION 2.1. A design $d \in D_0(v, b, k)$ is called a balanced test treatment incomplete block design (BTIBD) if the following conditions are satisfied:

1. d is incomplete.
2. There are constants λ_0 and λ_1 such that $\sum_{j=1}^{b} n_{d0j} n_{dij} = \lambda_0$, $1 \le i \le v$, and $\sum_{j=1}^{b} n_{di_1j} n_{di_2j} = \lambda_1$, $1 \le i_1 \ne i_2 \le v$.

The number n_{dij}, $0 \le i \le v$, $1 \le j \le b$, is the number of times that treatment i appears in block j under design d.

Such a design possesses a great amount of symmetry with respect to the test treatments and it can, indeed, be shown that $\mathrm{Var}_d(\hat{\tau}_i - \hat{\tau}_0)$ is independent of i, $1 \le i \le v$. Moreover, the information matrix for estimating the test treatment–control contrasts under such a design is a completely symmetric matrix [see Bechhofer and Tamhane (1981)]. This symmetry was utilized by Majumdar and Notz (1983) to obtain their main result. Before stating it, we need one more definition.

DEFINITION 2.2. By a BTIB$(v, b, k; t, s)$, we denote a design $d \in D_0(v, b, k)$ with the following properties:

1. d is a BTIBD.
2. There are s blocks in d each with $t + 1$ replications of the control, while each of the remaining $b - s$ blocks contains t replications of the control.
3. d is binary in the test treatments, i.e., $n_{dij} \in \{0, 1\}$ for $1 \le i \le v$, $1 \le j \le b$.

THEOREM 2.1 [Majumdar and Notz (1983)]. *If* $3 \le k \le v$, *then a* BTIB$(v, b, k; t, s)$ *is A-optimal if*

$$g(t, s) = \min\{g(x, z): (x, z) \in \Lambda\},$$

where

$$g(x, z) := (v-1)^2\big(bvk(k-1) - (bx+z)(vk-v+k) + (bx^2+2xz+z)\big)^{-1} + \big((bx+z)k - (bx^2+2xz+z)\big)^{-1}$$

and

$$\Lambda := \{(x, z): x \in \{0, 1, \dots, [k/2]-1\},\ z \in \{0, 1, \dots, b\} \text{ and } z > 0 \text{ if } x = 0\}$$

([$\cdot$] *denotes the largest integer function*).

In the remainder of this paper we will assume that the condition $3 \le k \le v$ is satisfied. We will also adopt the terminology from Hedayat and Majumdar (1984), where a BTIB$(v, b, k; t, s)$ is called a rectangular-type (R-type) design if

$s = 0$ or b and a step-type (S-type) design if $s \in \{1, \dots, b-1\}$. R-type designs are also known in the literature as augmented BIB (ABIB) designs. Through a more detailed study of the function g in Theorem 2.1, Hedayat and Majumdar (1985) obtained the following result on optimal R-type designs.

THEOREM 2.2. *A* BTIB$(v, b, k; 1, 0)$ *is A-optimal if*

$$(k-2)^2 + 1 \le v \le (k-1)^2.$$

The main result of this section is the following generalization of Theorem 2.2.

THEOREM 2.3. *A* BTIB$(v, b, k; t, 0)$ *is A-optimal if*

$$(k-t-1)^2 + 1 \le t^2 v \le (k-t)^2. \tag{2.1}$$

PROOF. By Theorem 2.1, it suffices to show that (2.1) implies that

$$g(t, 0) = \min\{g(x, z) \colon (x, z) \in \Lambda\}. \tag{2.2}$$

From Theorem 2.6 of Hedayat and Majumdar (1985), it follows that (2.2) holds if the following two conditions are satisfied:

$$\begin{aligned} &b(k-t)\big((k-2t-1)(v(k-1)-t)^2 - at^2(p-2t-1)\big) \\ &\quad \le v(k-2t-1)(p-2t-1)(k-1+(v-2)t) \end{aligned} \tag{2.3}$$

and

$$\begin{aligned} &b(k-t)\big(at^2(p-2t+1) - (k-2t+1)(v(k-1)-t)^2\big) \\ &\quad \le v(k-2t+1)(p-2t+1)(k-1+(v-2)t), \end{aligned} \tag{2.4}$$

where $a = (v-1)^2$ and $p = v(k-1) + k$. Since the right-hand sides in (2.3) and (2.4) are nonnegative, these inequalities are obviously satisfied if

$$(k-2t-1)(v(k-1)-t)^2 - at^2(p-2t-1) \le 0 \tag{2.5}$$

and

$$at^2(p-2t+1) - (k-2t+1)(v(k-1)-t)^2 \le 0. \tag{2.6}$$

The left-hand side in (2.5) equals $-vq_2(v)$, while that of (2.6) equals $vq_1(v)$, where

$$\begin{aligned} q_1(v) := {} &(k-1)t^2v^2 - \big((k-t-1)(k+t-1)(k-2t+1) + 2t^2(k-1)\big)v \\ &+ 2t(k-t-1)(k-2t+1) + t^2(k-1) \end{aligned}$$

and

$$\begin{aligned} q_2(v) := {} &(k-1)t^2v^2 - \big((k-t-1)(k+t-1)(k-2t-1) + 2t^2(k-1)\big)v \\ &+ 2t(k-t-1)(k-2t-1) + t^2(k-1). \end{aligned}$$

Hence, (2.5) and (2.6) are equivalent to $q_2(v) \ge 0$ and $q_1(v) \le 0$. Since both q_1

and q_2 are convex functions in v, to establish the validity of Theorem 2.3 it suffices to show that

(i) $q_1(1) \le 0$,
(ii) $q_2(1) \le 0$,
(iii) $q_1((k-t)^2/t^2) \le 0$,
(iv) $q_2(((k-t-1)^2+1)/t^2) \ge 0$.

A simple evaluation gives us that

$$q_1(1) = -(k-t-1)^2(k-2t+1) \le 0,$$

which shows (i). Also

$$q_2(1) = -(k-t-1)^2(k-2t-1) \le 0.$$

This shows (ii). Further, we obtain that

$$q_1\big((k-t)^2/t^2\big) = \big((-2t+1)k^3 + (6t^2-1)k^2 - (t^4+6t^3+3t^2-2t)k + 2t^5 + 3t^4 - t^2\big)/t^2.$$

Since $k \ge 2t$ and since the right-hand side in the preceding equality, viewed as a function of k, is decreasing on $(2t, \infty)$, it follows by replacing k by $2t$ that

$$q_1\big((k-t)^2/t^2\big) \le -(t-1)^2 \le 0,$$

establishing (iii).

Finally,

$$q_2\Big(\big((k-t-1)^2+1\big)/t^2\Big) = \Big((k-2t-1)\big((k-1)^2 - t^4 + t^2\big) + k - 1\Big)/t^2.$$

To see that this is nonnegative, we merely notice that $k \le v \le (k-t)^2/t^2$ implies that $k \ge t^2 + t$. This shows (iv) and completes the proof of Theorem 2.3. □

We would like to point out that it can be shown that, for fixed k and t, at most one value of v which satisfies (2.3) and (2.4) for all $b \ge v$ is not covered by the relation (2.1).

The result of Theorem 2.3 enables us also to obtain large families of A-optimal R-type designs from families of BIB designs. We formalize this in Corollary 2.1 and give an example of its use in Corollary 2.2. Other examples can be found in Stufken (1986a).

COROLLARY 2.1. *If there are a* BIBD(v, b, k) *and an integer*

$$t \in \{1, 2, \ldots, k-1\}$$

such that

(i) $v \geq k + t$ *and*
(ii) $(k-1)^2 + 1 \leq t^2 v \leq k^2$,

then an A-optimal BTIB$(v, b, k + t; t, 0)$ *exists.*

The proof is a simple verification of (2.1). For parameters satisfying the conditions in this corollary, the result gives a formal justification for an idea of Cox (1958), who first recommended the use of R-type designs.

COROLLARY 2.2. *If λ is a perfect square and $v \geq k + \lambda^{1/2}$, then a symmetric* BIBD(v, k, λ) *can be embedded in an A-optimal* BTIB$(v, v, k + \lambda^{1/2}; \lambda^{1/2}, 0)$.

PROOF. We verify the conditions in Corollary 2.1. It is easy to verify that $\lambda^{1/2} \leq k - 1$ under the assumptions in Corollary 2.2. Condition (i) is satisfied by assumption, while (ii) can be seen from

$$\lambda v = \lambda(v-1) + \lambda = k(k-1) + \lambda \leq k^2$$

and

$$\lambda v \geq k(k-1) \geq (k-1)^2 + 1. \qquad \square$$

We conclude this section by giving a table with all A-optimal BTIB$(v, b, k; t, 0)$ designs, $3 \leq k \leq 10$, $k \leq v \leq 30$, whose A-optimality follows from Theorem 2.3 (see Table 1). The given values of b in the table may be replaced by any multiple of the given number. The BIB$(v, b, k - t)$ needed for the construction of the given BTIB exists for all parameters. Most of them, or their complements, can be found in Hall [(1986), Table 1.1].

3. A-optimal S-type designs. Families of A-optimal S-type designs are, with one exception in Cheng, Majumdar, Stufken and Ture (1986), not available in the literature. The reason for this is twofold. Partly, it is due to the fact that a characterization of families of parameters corresponding to S-type designs whose A-optimality can be concluded from Theorem 2.1 is harder than the analogue for optimal R-type designs. In addition, once a family of such parameters has been established, we will still have to answer the often difficult combinatorial question regarding their existence by giving a method for their construction. In the case of R-type designs, we could refer to the available literature on BIB designs; for S-type designs, such an easy way out is not available. Cheng, Majumdar, Stufken and Ture (1986) proved a useful result for the determination of families of parameters of A-optimal S-type designs. A formulation of their result is

THEOREM 3.1. *With $g(x, z)$ and Λ as in Theorem* 2.1, *if for some* $t \in \{0, 1, \ldots, [k/2] - 1\}$, $s \in \{1, 2, \ldots, b - 1\}$,

$$g(t, s) \leq \min\{g(t, s-1), g(t, s+1)\}, \tag{3.1}$$

TABLE 1
A-optimal BTIB(v, b, k; t, 0) *designs*, $3 \le k \le 10$, $k \le v \le 30$

No.	v	b	k	t	No.	v	b	k	t
1	3	3	3	1	20	15	15	10	2
2	4	6	3	1	21	15	105	5	1
3	5	10	4	1	22	16	20	5	1
4	6	10	4	1	23	16	30	10	2
5	7	7	4	1	24	17	68	6	1
6	8	28	8	2	25	18	306	6	1
7	8	56	4	1	26	19	171	6	1
8	9	12	4	1	27	20	76	6	1
9	9	12	8	2	28	21	21	6	1
10	10	15	5	1	29	22	462	6	1
11	10	30	9	2	30	23	253	6	1
12	11	55	5	1	31	24	552	6	1
13	11	55	9	2	32	25	30	6	1
14	12	33	5	1	33	26	65	7	1
15	12	132	9	2	34	27	117	7	1
16	13	13	5	1	35	28	126	7	1
17	13	39	10	2	36	29	406	7	1
18	14	91	5	1	37	30	145	7	1
19	14	91	10	2					

then

$$g(t, s) = \min\{g(x, z): (x, z) \in \Lambda\}.$$

This result can be used if we determine parameters for which (3.1) is satisfied and for which we can then show the existence of the corresponding S-type design. Cheng, Majumdar, Stufken and Ture (1986) showed, proceeding in this manner, that an A-optimal

$$\mathrm{BTIB}\big(k^2 - 1, \gamma(k+2)(k^2-1), k; 0, \gamma(k+1)(k^2-1)\big)$$

exists if k is a prime or power of a prime, where γ is any positive integer. In this section, we will derive families of parameters which satisfy (3.1) for the case $t = 0$. They will include the preceding result. We will then conclude this section with a patchwork construction for designs with the obtained parameters. Let us start by looking at $g(0, z)$, $z \in (0, b]$. It is not hard to show that this function attains its minimum either at b or, assuming $v \ge 4$, at

$$z_0 := bk\big((v-1)(v+1)^{1/2} - (v+1)\big)/(v+1)(v-3) \tag{3.2}$$

if $z_0 < b$.

We are interested in the latter case. It can be verified that $z_0 < b$ if and only if $v \ge (k-1)^2 + 1$. Thus, if this condition holds, we define $s = [z_0]$ or $s = [z_0] + 1$ depending on which of the two gives a smaller value for $g(0, z)$. With this choice of s, condition (3.1) will be satisfied, implying that a

BTIB$(v, b, k; 0, s)$ is A-optimal, if it exists. This observation is useful if a particular choice of v, b and k is under consideration. It is then easy to obtain s and an attempt can be made to construct the desired optimal S-type design. A useful first step in such an attempt is to verify whether the necessary conditions for the existence of a BTIB$(v, b, k; 0, s)$ are satisfied. These are [see also Hedayat and Majumdar (1984)]

$$(k-1)s \equiv 0 \pmod{v}, \tag{3.3}$$

$$k(b-s) \equiv 0 \pmod{v}, \tag{3.4}$$

$$(k-2)(k-1)s/v + (k-1)k(b-s)/v \equiv 0 \pmod{v-1}. \tag{3.5}$$

If one or more of these conditions are violated or the nonexistence of the desired design is obtained through some other argument, considerations as in Cheng, Majumdar, Stufken and Ture (1986) may lead to an A-optimal or highly efficient design in $D_0(v, b, k)$.

For the purpose of deriving families of optimal S-type designs, the form of s is rather complicated. The problem is made more tractable if we make the additional assumption that z_0 is an integer and, thus, $s = z_0$. A design that will be obtained under this assumption has the extra feature that any number of copies of it form again an A-optimal design. It is unknown whether this is true in general. The following result characterizes all parameters of interest for which z_0 is an integer in $\{1, \dots, b-1\}$.

THEOREM 3.2. *The parameters for which $z_0 \in \{1, \dots, b-1\}$ and for which the necessary conditions* (3.3), (3.4) *and* (3.5) *are satisfied are given by*

$$v = \alpha^2 - 1, \qquad k = \beta, \qquad b = \gamma\alpha(\alpha+2)(\alpha^2-1)/\delta\varepsilon,$$

where $\alpha \geq \beta \geq 3$, $\delta = \gcd(\beta, \alpha(\alpha+2))$, $\varepsilon = \gcd(\beta\delta^{-1}, \alpha^2 - 1)$ and γ is an arbitrary positive integer. [*By* $\gcd(a, b)$, *we denote the greatest common divisor of the integers a and b.*]

PROOF. For z_0 to be an integer, $v + 1$ must be a perfect square, say $v = \alpha^2 - 1$. Let $k = \beta \geq 3$. For $z_0 < b$, it must be that $v \geq (k-1)^2 + 1$, or $\alpha \geq \beta$. From (3.2), we obtain now $z_0 = b\beta(\alpha+1)/\alpha(\alpha+2)$. Since $\gcd(\alpha+1, \alpha(\alpha+2)) = 1$, we see that this is an integer only if $b \equiv 0 \pmod{\alpha(\alpha+2)/\delta}$. If we set $b = \gamma_1\alpha(\alpha+2)/\delta$, we obtain with $s = z_0$ from (3.3) and (3.4) [which imply $kb - s \equiv 0 \pmod{v}$] that $\gamma_1\beta(\alpha^2 + \alpha - 1)/\delta \equiv 0 \pmod{\alpha^2 - 1}$ or, equivalently, $\gamma_1\beta/\delta \equiv 0 \pmod{\alpha^2-1}$. Therefore, $\gamma_1 = \gamma(\alpha^2-1)/\varepsilon$ for some positive integer γ. This gives the parametrization for b as asserted in the theorem. It can indeed easily be verified that (3.3), (3.4) and (3.5) are now satisfied, while $z_0 = s = \gamma\beta(\alpha+1)(\alpha^2-1)/\delta\varepsilon$, which is indeed an integer. □

This result tells us thus that a

$$\mathrm{BTIB}\big(\alpha^2 - 1, \gamma\alpha(\alpha+2)(\alpha^2-1)/\delta\varepsilon, \beta; 0, \gamma\beta(\alpha+1)(\alpha^2-1)/\delta\varepsilon\big)$$

is A-optimal for any α, β, γ, δ and ε as in Theorem 3.2. Although the conditions

(3.3), (3.4) and (3.5) are also satisfied, this does unfortunately not guarantee the existence of the design. Patchwork constructions may resolve this problem, either for individual designs or for certain families of designs of the preceding form. We give here one example of such a construction. Let $\alpha = \beta = k$. This results in a

$$\mathrm{BTIB}\big(k^2 - 1, \gamma(k + 2)(k^2 - 1), k; 0, \gamma(k + 1)(k^2 - 1)\big),$$

the existence of which was shown for k a prime or power of a prime, as referred to earlier. We add to this the following result.

THEOREM 3.3. *An A-optimal* BTIB$(k^2 - 1, \gamma(k + 2)(k^2 - 1), k; 0, \gamma(k + 1)(k^2 - 1))$ *exists if* $k + 1$ *is a prime or power of a prime.*

PROOF. It suffices to show the existence for $\gamma = 1$. The layout of the desired design is as follows:

<table>
<tr><td></td><td>$(k + 1)(k^2 - 1)$</td><td>$k^2 - 1$</td><td></td></tr>
<tr><td>1</td><td>control</td><td rowspan="2">B</td><td rowspan="2">k</td></tr>
<tr><td>$k - 1$</td><td>A</td></tr>
</table>

We have to determine the parts labeled by A and B. Start by partitioning the $k^2 - 1$ test treatments into $k - 1$ groups $G_1, \dots, G_{k-1}$ of cardinality $k + 1$ each. For each of these groups G_i form the trivial BIBD, with blocks consisting of all subsets of G_i of cardinality k. This gives a total of $k^2 - 1$ blocks of size k, blocks that we use to form B. Next form an orthogonal array $OA((k + 1)^2, k - 1, k + 1, 2)$ of index unity. The construction of this array is well known if $k + 1$ is a prime or power of a prime, which is just our assumption. [Actually an $OA((k + 1)^2, k + 2, k + 1, 2)$ can even be constructed under our assumption. See, e.g., Bose and Bush (1952).] Use this orthogonal array to construct a group divisible design with $k^2 - 1$ treatments in blocks of size $k - 1$ in which the treatments are partitioned in $k - 1$ groups and a pair of treatments from the same group does not appear at all, while treatments from distinct groups appear exactly once as a pair. Clearly we can arrange this such that the groups are again $G_1, \dots, G_{k-1}$. Take $k - 1$ replications of this group divisible design and let this be A. It is easy to verify that the design constructed in this way is the desired S-type design. □

As an example, we will illustrate the preceding construction for $k = 3$. Let $G_1 = \{1, 2, 3, 4\}$ and $G_2 = \{5, 6, 7, 8\}$. The part labeled by B is then formed by the following eight blocks:

1	1	1	2	5	5	5	6
2	2	3	3	6	6	7	7
3	4	4	4	7	8	8	8

We use the following $OA(16, 2, 4, 2)$ based on the symbols a, b, c and d:

$$\begin{array}{cccccccccccccccc} a & a & a & a & b & b & b & b & c & c & c & c & d & d & d & d \\ a & b & c & d & a & b & c & d & a & b & c & d & a & b & c & d \end{array}$$

Make a one-to-one correspondence between $\{a, b, c, d\}$ and G_i, for $i = 1, 2$. Use this correspondence to replace the symbols in the ith row of the orthogonal array by the elements of G_i. This could, for example, lead to the following 2×16 array:

$$\begin{array}{cccccccccccccccc} 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 & 4 & 4 & 4 & 4 \\ 5 & 6 & 7 & 8 & 5 & 6 & 7 & 8 & 5 & 6 & 7 & 8 & 5 & 6 & 7 & 8 \end{array}$$

View the preceding as 16 blocks of size 2 and take 2 replications of each of these blocks. The resulting 32 blocks are used to form the part labeled by A.

Several other patchwork constructions for individual designs can be found in Stufken (1986a).

4. Concluding remarks. The results in Section 2 extend the main results of Hedayat and Majumdar (1985). Theorem 2.3 and Corollary 2.1 provide a sufficient condition for the A-optimality of R-type designs, a condition that can easily be verified. Large families of optimal R-type designs can be obtained from it. It is unfortunately known that for many families of parameters v, b and k the best design is not an R-type design. An alternative would then be to search among S-type designs. Section 3 gives some families of optimal S-type designs and some ideas for finding optimal designs for specified parameters. The construction of these S-type designs is usually a nontrivial problem. Patching BIB designs and/or group divisible designs together in an appropriate way may resolve problems of this kind. After these considerations, there will still be many parameters v, b and k for which no optimal design has been found. This will be the case if optimal designs are neither of the R-type nor S-type or if Theorem 2.1 is not strong enough to determine their optimality. In such cases, one could either search for highly efficient R-type designs [see Stufken (1986b)] or give consideration to the ideas suggested in Cheng, Majumdar, Stufken and Ture (1986).

We finally point out that all the optimal designs derived in this paper are not only A-optimal, but also MV-optimal. This means that these designs minimize

$$\max_{1 \le i \le v} \operatorname{Var}_d(\hat{\tau}_i - \hat{\tau}_0)$$

over all designs $d \in D_0(v, b, k)$.

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