Statistica Sinica **5**(1995), 605-615

EFFICIENT BLOCK DESIGNS IN THE PRESENCE OF TRENDS

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Abstract. The problem of identifying and constructing optimal and efficient block designs for comparing several treatments in the presence of (possibly different) linear trends within the blocks is studied. Special emphasis is on efficient designs within the classes of binary and trend-free designs.

Key words and phrases: Binary designs, BIB design, difference set, semibalanced array, trend-free designs, universally optimal designs, Youden design.

1. Introduction

We consider the problem of comparing v treatments on experimental units that are divided into b blocks of k units each. The units within each block are equispaced over time or space. Aside from the treatment and block effects, observations within blocks are also influenced by a trend. The problem is to identify designs that are efficient for these experiments.

Bradley and Yeh (1980) first studied the problem of constructing block designs that are "trend-free". This was followed by several papers (see Lin and Dean (1991) for a bibliography). A feature of the models in the existing literature is that the trend is assumed to be the same in each block. Even though it is realistic in many experiments, this assumption may be difficult to justify when the blocks are substantially dissimilar. In agricultural experiments, for example, the blocks may be located in fields that are far apart, with different fertility gradients.

In this paper we consider models in which different blocks can have different trends. Our goal is to identify efficient designs for these models. Besides considering trend-free designs, we also study the performance of binary designs. The latter, it will be seen, are not trend-free. Nevertheless, binary designs are important for at least two reasons. One is that these designs are expected to perform well when the trend is weak or if there truly is a common trend in all blocks. The other is the familiarity that experimenters have with binary designs due to their wide usage.

In Section 2 we state the model explicitly and derive the information matrix. Optimal binary designs are identified in Section 3 and optimal trend-free designs in Section 4. In Section 5 we compute the efficiency of optimal designs in Sections 3 and 4 in the class of all designs, as well as identify some optimal designs in the latter class when $k = 3$.

2. The Model

A design determines the assignment of treatments to the periods within the blocks. If a design d assigns treatment i $(0 \le i \le v-1)$ to period ℓ $(1 \le \ell \le k)$ of block j $(1 \le j \le b)$, then we write $d(\ell, j) = i$. For the observation $y_{\ell j}$ at period ℓ of block j, we consider the model

$$y_{\ell j} = \mu + \tau_{d(\ell,j)} + \beta_j + \sum_{\alpha=1}^{p_j} \phi_\alpha(\ell)\theta_{j\alpha} + e_{\ell j} \tag{2.1}$$

where τ, β and θ are the treatment, block and trend parameters, respectively, ϕ_α is the orthogonal polynomial of degree α on $1, \cdots, k$ and p_j $(0 \le p_j \le k-1)$ is the degree of the trend in block j. The error e has the properties $E(e_{\ell j}) = 0$, $\text{var}(e_{\ell j}) = \sigma^2$, $\text{cov}(e_{\ell j}, e_{\ell' j'}) = 0$ if $(\ell, j) \ne (\ell', j')$. The difference between (2.1) and the model of Bradley and Yeh (1980, equation (2.3)) is that here the trend parameter $\theta_{j\alpha}$ depends on the block j.

A design d will be represented by a $k \times b$ array with entries from $\{0, 1, \ldots, v-1\}$, the rows representing periods and the columns blocks. A design d is said to be connected under model (2.1) provided all treatment differences of the form $\tau_p - \tau_q$ are estimable. Let

$$\begin{aligned}\mathcal{D}(v, b, k) = \{&\text{all } k \times b \text{ arrays with entries from } \{0, 1, \ldots, v-1\}\\ &\text{which are connected}\}.\end{aligned}$$

The model (2.1) is quite involved since it has several nuisance parameters. In this paper we only consider a linear trend in each block, i.e. $p_j = 1$ for all $j = 1, \ldots, b$. Writing θ_j for θ_{j1}, the model reduces to:

$$y_{\ell j} = \mu + \tau_{d(\ell,j)} + \beta_j + \phi_1(\ell)\theta_j + e_{\ell j}. \tag{2.2}$$

Here θ_j is the slope of the trend line in block j. Though most of the results are quite general, our principal focus is on experiments with $k \le v$.

For $d \epsilon \mathcal{D}(v, b, k)$, let

$$\delta^i_{\ell j} = \delta^i_{\ell j}(d) = \begin{cases} 1, & \text{if } d(\ell, j) = i, \\ 0, & \text{otherwise.} \end{cases}$$

Let $n_{dij} = \sum_{\ell=1}^{k} \delta_{\ell j}^{i}$, $s_{di\ell} = \sum_{j=1}^{b} \delta_{\ell j}^{i}$, $N_d = (n_{dij})$, a $v \times b$ matrix, $r_{di} = \sum_{j=1}^{b} n_{dij}$ and $R_d = \mathrm{diag}(r_{d0}, \ldots, r_{d,v-1})$. Further, let $h_{dij} = \sum_{\ell=1}^{k} \delta_{\ell j}^{i} \phi_1(\ell)$ and $H_d = (h_{dij})$, a $v \times b$ matrix. Then it can be seen that the information matrix for the treatment effects $(\tau_0, \tau_1, \ldots, \tau_{v-1})$ is:

$$C_d = R_d - (1/k) N_d N_d' - H_d H_d'. \tag{2.3}$$

If $\theta_j = 0$ for $j = 1, \ldots, b$ in (2.2), then the information matrix reduces to $C_{bd} = R_d - (1/k) N_d N_d'$, the information matrix for the additive model with treatments and blocks only. Hence

$$C_d = C_{bd} - H_d H_d'. \tag{2.4}$$

Throughout the sequel, let $H_d H_d' = G_d = (g_{dii'})$ where, for treatments i and i', $g_{dii'} = \sum_{j=1}^{b} h_{dij} h_{di'j}$.

We use the universal optimality criterion of Kiefer (1975) to derive optimal designs in various subsets of $\mathcal{D}(v, b, k)$. A design d^* is universally optimal whenever C_{d^*} is completely symmetric (c.s.) and $\mathrm{tr}\, C_{d^*}$ is a maximum in the set of designs under consideration. For a design d with c.s. C_d, we define the efficiency of d as:

$$e(d) = \mathrm{tr}\, C_d / \max_{d_1 \in \mathcal{D}(v,b,k)} \mathrm{tr}\, C_{d_1} \tag{2.5}$$

Comment. The above measure is motivated by the following considerations. We would like to define efficiency of a given design d as $e_0(d) = \mathrm{tr}\, C_{d_0}^{+} / \mathrm{tr}\, C_d^{+}$ where A^{+} denotes the Moore-Penrose inverse of A and d_0 minimizes $\mathrm{tr}\, C_{d_o}^{+}$ over $d \in D(v, b, k)$. It is easy to see that $\mathrm{tr}\, C_{d_0}^{+} \geq (v-1)^2 / \mathrm{tr}\, C_{d_0} \geq (v-1)^2 / \mathrm{tr}\, C_{d_1}$ where d_1 maximizes $\mathrm{tr}\, C_d$ over $d \in D(v, b, k)$. Further, if C_d is c.s., $\mathrm{tr}\, C_d^{+} = (v-1)^2 / \mathrm{tr}\, C_d$. Thus

$$e_0(d) = \mathrm{tr}\, C_{d_0}^{+} / \mathrm{tr}\, C_d^{+} \geq \mathrm{tr}\, C_d / \mathrm{tr}\, C_{d_1} = e(d)$$

and $e(d)$ provides us with a lower bound for the true efficiency $e_0(d)$. It is clearly easier to obtain $\max\, \mathrm{tr}\, C_d$ than $\min\, \mathrm{tr} C_d^{+}$.

3. Efficient Binary Designs

A design d is called binary if the block design (with columns as blocks) is binary, i.e., $n_{dij} \in \{0, 1\}$ for all i, j. Let

$$\mathcal{D}_b(v, b, k) = \{d \in \mathcal{D}(v, b, k) :\ n_{dij} \in \{0, 1\},\ i = 0, 1, \ldots, v-1;\ j = 1, \ldots, b\}.$$

We shall identify some designs in $\mathcal{D}_b(v, b, k)$ that have a completely symmetric information matrix with maximal trace, i.e. designs that are universally optimal among binary designs.

For a $d \in \mathcal{D}_b(v,b,k)$, it follows from (2.4) that

$$\begin{aligned}\operatorname{tr} C_d = b(k-1) - \operatorname{tr} G_d &= b(k-1) - \sum_{i=0}^{v-1}\sum_{j=1}^{b}(\sum_{\ell=1}^{k}\delta_{\ell j}^{i}\phi_1^2(\ell))\\ &= b(k-1) - \sum_{i=0}^{v-1}\sum_{\ell=1}^{k} s_{di\ell}\phi_1^2(\ell) = b(k-2),\end{aligned}$$

that is, designs in $\mathcal{D}_b(v,b,k)$ have constant $\operatorname{tr} C_d$.

One way to obtain a c.s. C_d is to choose a Balanced Incomplete Block (BIB) design in $\mathcal{D}_b(v,b,k)$ with c.s. G_d. This method has the advantage that it is model robust in the sense that the design is highly efficient when the trend is absent or very weak. It is not clear whether or not this is the only way to obtain a d in $\mathcal{D}_b(v,b,k)$ with C_d c.s..

The diagonal entries g_{dii} of G_d are equal if and only if

$$g_{dii} = b/v, \quad i = 0, 1, \ldots, v-1, \tag{3.1}$$

since $\operatorname{tr} G_d = b$. Condition (3.1) is satisfied whenever d is a Youden design, i.e., a BIB design having each treatment occurring in each of periods $1, \ldots, k$ the same number of times.

For $i \neq i'$,

$$g_{dii'} = \sum_{j=1}^{b} h_{dij}h_{di'j} = \sum_{j=1}^{b}\sum_{\ell=1}^{k}\sum_{\substack{\ell'=1\\ \ell'\neq\ell}}^{k} \delta_{\ell j}^{i}\delta_{\ell' j}^{i'}\phi_1(\ell)\phi_1(\ell').$$

Let us define

$$m_{d\ell\ell'}^{ii'} = \sum_{j=1}^{b}\delta_{\ell j}^{i}\delta_{\ell' j}^{i'},$$

the number of columns of d that have i in row ℓ and i' in row ℓ'. Clearly,

$$g_{dii'} = \sum_{\ell=1}^{k}\sum_{\ell<\ell'}^{k}\phi_1(\ell)\phi_1(\ell')[m_{d\ell\ell'}^{ii'} + m_{d\ell'\ell}^{ii'}].$$

Since the row sums of G_d are zero, it follows from (3.1) that G_d is completely symmetric if and only if

$$g_{dii'} = -b/(v(v-1)) \quad \text{for } i \neq i'. \tag{3.2}$$

Lemma 3.1. *A necessary condition for a* BIB *design in* $\mathcal{D}_b(v,b,k)$ *to have a c.s.* G_d *is:*

$$bk(k^2-1) \equiv \begin{cases} 0 \pmod{3v(v-1)}, & \text{if } k \text{ is even},\\ 0 \pmod{12v(v-1)}, & \text{if } k \text{ is odd}.\end{cases}$$

Proof. If k is even, $\phi_1(\ell) = \phi_1^*(\ell)/(k(k^2-1)/3)^{1/2}$ with $\phi_1^*(\ell) \in \boldsymbol{Z}$, where

$$\boldsymbol{Z} = \{\ldots, -3, -2, -1, 0, 1, 2, 3, \ldots\}.$$

From (3.2) it follows that $(b/(v(v-1)))(k(k^2-1)/3) \in \boldsymbol{Z}$.

If k is odd, the result follows in the same way since $\phi_1(\ell) = \phi_1^*(\ell)/(k(k^2-1)/12)^{1/2}$ with $\phi_1^*(\ell) \in \boldsymbol{Z}$.

Example 3.1. Let $v = 7$ and $k = 3$. From Lemma 3.1 it follows that $b \equiv 0 \pmod{21}$. A universally optimal design in $\mathcal{D}_b(7, 21, 3)$ is:

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 0 & 4 & 5 & 6 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 6 & 0 & 1 \\ 2 & 3 & 4 & 5 & 6 & 0 & 1 & 1 & 2 & 3 & 4 & 5 & 6 & 0 & 4 & 5 & 6 & 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 6 & 0 & 1 & 1 & 2 & 3 & 4 & 5 & 6 & 0 \end{pmatrix}.$$

We now give one well known method for constructing universally optimal designs in classes $\mathcal{D}_b(v, b, k)$. Let d be a BIB (v, b, r, k, λ) design. The matrix G_d is c.s., i.e. (3.2) is satisfied, if for all $\ell \neq \ell'$, $i \neq i'$,

$$m_{d\ell\ell'}^{ii'} + m_{d\ell'\ell}^{ii'} = \alpha, \tag{3.3}$$

a constant. Designs with property (3.3) were introduced by Rao (1961), who called them "orthogonal arrays of type II", and later (Rao (1973)) renamed them "semibalanced arrays". These are also related to "perpendicular arrays" of Lindner (1988). It is easy to see that a design satisfying (3.3) is a BIB design with columns as blocks. Semibalanced arrays have been used by several authors, such as Morgan and Chakravarti (1988), Cheng (1988) and Martin and Eccleston (1991) to design experiments with correlated observations. The design given in Example 3.1 is a semibalanced array.

For construction of semibalanced arrays see Rao (1961) and Mukhopadhyay (1972). It is known, for example, that when v or k is a power of a prime, these arrays can be constructed. Here is an example.

Example 3.2. Let $v = 5$ and $k = 4$. The following is a semibalanced array with $m_{d\ell\ell'}^{ii'} + m_{d\ell'\ell}^{ii'} = 1$ for all $\ell \neq \ell'$, $i \neq i'$. Hence it is universally optimal in $\mathcal{D}_b(5, 10, 4)$.

$$\begin{matrix} 1 & 2 & 2 & 3 & 3 & 4 & 4 & 0 & 0 & 1 \\ 2 & 4 & 3 & 0 & 4 & 1 & 0 & 2 & 1 & 3 \\ 3 & 1 & 4 & 2 & 0 & 3 & 1 & 4 & 2 & 0 \\ 4 & 3 & 0 & 4 & 1 & 0 & 2 & 1 & 3 & 2 \end{matrix}$$

At present, the authors do not know of any other optimal designs in classes $\mathcal{D}_b(v, b, k)$ which are not semibalanced arrays or permutations of semibalanced arrays.

4. Efficient Trend-Free Designs

A design d may be called *trend-free* if the presence of a trend results in no loss of information, that is, $C_d = C_{bd}$. But from (2.4), this last equality occurs if and only if for $H_d = (h_{dij})$,

$$h_{dij} = 0 \quad \text{for} \quad i = 0, 1, \ldots, v-1, \quad j = 1, \ldots, b. \tag{4.1}$$

For the remainder of this paper, let

$$\mathcal{D}_{tf}(v,b,k) = \{d \in \mathcal{D}(v,b,k) : h_{dij} = 0 \quad \text{for} \quad i = 0, 1, \ldots, v-1, \quad j = 1, \ldots, b\}.$$

Condition (4.1) is the same as

$$\sum_{\ell=1}^{k} \delta_{\ell j}^{i} \phi_1(\ell) = 0, \quad i = 0, 1, \ldots, v-1. \tag{4.2}$$

Since $\phi_1(\ell) = c(\ell - (k+1)/2)$ for a normalizing constant c,

$$\sum_{\ell=1}^{k} \delta_{\ell j}^{i} \ell = n_{dij}(k+1)/2.$$

Clearly, from this last expression, a binary design cannot be trend-free. A necessary condition that d is trend-free is:

$$n_{dij}(k+1) \equiv 0 \,(\bmod\, 2), \quad i = 0, 1, \ldots, v-1; \; j = 1, \ldots, b. \tag{4.3}$$

A sufficient, though not necessary, condition for (4.2) is:

$$\delta_{\ell j}^{i} = \delta_{(k-\ell+1),j}^{i}, \quad \ell = 1, \ldots, \lfloor k/2 \rfloor, j = 1, \ldots, b, i = 0, 1, \ldots, v-1 \tag{4.4}$$

where $\lfloor a \rfloor$ denotes the greatest integer not exceeding $a > 0$.

For $d \in \mathcal{D}_{tf}(v,b,k)$,

$$\operatorname{tr} C_d = bk - (1/k) \sum_{j=1}^{b} \sum_{i=0}^{v-1} n_{dij}^2.$$

To maximize the trace, therefore, one has to minimize $\sum_{j=1}^{b} \sum_{i=0}^{v-1} n_{dij}^2$. We will identify universally optimal designs in $\mathcal{D}_{tf}(v,b,k)$ separately for the two cases: k even and k odd.

Case I: k even. For $d \in \mathcal{D}_{tf}(v,b,k)$, it follows from (4.3) that $n_{dij} \in \{0, 2, 4, \ldots\}$. Clearly, d maximizes $\operatorname{tr} C_d$ if

$$n_{dij} \in \{0, 2\}, \quad i = 0, 1, \ldots, v-1, \quad j = 1, \ldots, b.$$

To get a c.s. C_d, it is sufficient to consider designs of the form $d = (d_1, d_2)^T$ with $n_{d_1ij} = n_{d_2ij} \in \{0, 1\}$ such that (4.4) holds for d and $C_{bd_1} = (1/2)C_{bd}$ is c.s.. This leads to the following theorem.

Theorem 4.1. *Let k be even. Let $d_0 \in \mathcal{D}(v, b, k/2)$ be any design such that the columns form a* $\mathrm{BIB}(v, b, r, k/2, \lambda)$ *design and let d_0^{-1} be d_0 with rows ℓ and $(k/2) - \ell + 1$ interchanged for each $\ell = 1, \ldots, k/2$. Then the $k \times b$ array $d^* = (d_0, d_0^{-1})^T$ is universally optimal in $\mathcal{D}_{tf}(v, b, k)$.*

For the designs d^* given in Theorem 4.1, we have

$$\max_{d \in \mathcal{D}_{tf}(v,b,k)} \operatorname{tr} C_d = \operatorname{tr} C_{d^*} = 2 \operatorname{tr} C_{bd_0} = 2b(k/2 - 1) = b(k-2) = \max_{d \in \mathcal{D}_b(v,b,k)} \operatorname{tr} C_d.$$

Thus, the universally optimal trend-free and binary designs are equally efficient when k is even! The optimal trend-free design d^*, having fewer combinatorial restrictions, is expected to exist more often than a universally optimal binary design of Section 3. On the other hand, a binary design has some attractions, such as model robustness, as we have mentioned in Sections 1 and 3.

Case II: k odd. Let $k = 2q - 1$.

Lemma 4.1. *For $k = 2q - 1$, a design d in $D_{tf}(v, b, k)$ has maximal $\operatorname{tr} C_d$ in $D_{tf}(v, b, k)$ if and only if for each $j = 1, \ldots, b$,*

$$\delta^i_{qj} = 1 \Rightarrow n_{dij} = 1 \quad \textit{and} \quad \delta^i_{qj} = 0 \Rightarrow n_{dij} \in \{0, 2\}.$$

Proof. Since $\phi_1(q) = 0$, (4.2) is:

$$\sum_{\ell=1}^{q-1} \delta^i_{\ell j} \phi_1(\ell) + \sum_{\ell=q+1}^{k} \delta^i_{\ell j} \phi_1(\ell) = 0.$$

It follows that, for $\ell \neq q$, if $\delta^i_{\ell j} = 1$, then $n_{dij} \geq 2$, and if $\delta^i_{qj} = 1$, then $n_{dij} - \delta^i_{qj} \in \{0, 2, \ldots, k\}$. Suppose $\delta^i_{qj} = 1$ and $n_{dij} - \delta^i_{qj} = t \geq 2$. In column j, if we replace symbol i in all rows except q by a symbol i' which does not appear in column j (we can do this since $k \leq v$), then the new column j has a smaller value of $\sum_{i=1}^v n^2_{dij}$ than the old column j since $n^2_{dij} + n^2_{di'j}$ is $1 + t^2$ in the new column j but it is $(1+t)^2$ in the old column j and $(1+t)^2 > 1 + t^2$. Hence the lemma.

If we write $d \in \mathcal{D}_{tf}(v, b, k)$ as $d = (d_1, d_0, d_2)^T$, where d_0 is $1 \times b$, $N_{d_1} = N_{d_2}$ and $\delta^i_{\ell j}(d) = \delta^i_{(k-\ell+1),j}(d)$ for $\ell = 1, \ldots, q-1$, then $C_d = C_{bd} = R_d - N_d N'_d = R_d - (2N_{d_1} + N_{d_0})(2N_{d_1} + N_{d_0})'$. This leads to the following theorem.

Theorem 4.2. *Let $k = 2q - 1$. Let $d_1 \in \mathcal{D}(v, b, q-1)$ be a design whose columns form a* $\mathrm{BIB}(v, b, r, q-1, \lambda)$ *design, and let $d_0 \in \mathcal{D}(v, b, 1)$ be such that the columns* *of* $\binom{d_1}{d_0}$ *form a* BIB(v, b, r', q, λ') *design. Let* d_1^{-1} *be* d_1 *with rows* ℓ *and* $q - \ell$ *interchanged for each* $\ell = 1, \ldots, q-1$. *Then the* $k \times b$ *array* $d^* = (d_1, d_0, d_1^{-1})^\top$ *is universally optimal in* $\mathcal{D}_{tf}(v, b, k)$.

Example 4.1. Let $v = 7$ and $k = 3$. The following design is optimal in $\mathcal{D}_{tf}(7, 21, 3)$:

$$\begin{pmatrix} 1 & 1 & 1 & 5 & 6 & 7 & 2 & 2 & 2 & 6 & 7 & 3 & 3 & 3 & 7 & 4 & 4 & 4 & 5 & 5 & 6 \\ 2 & 3 & 4 & 1 & 1 & 1 & 3 & 4 & 5 & 2 & 2 & 2 & 5 & 6 & 3 & 5 & 6 & 7 & 6 & 7 & 7 \\ 1 & 1 & 1 & 5 & 6 & 7 & 2 & 2 & 2 & 6 & 7 & 3 & 3 & 3 & 7 & 4 & 4 & 4 & 5 & 5 & 6 \end{pmatrix}.$$

Example 4.2. Let $v = 5$ and $k = 5$. The following design is optimal in $\mathcal{D}_{tf}(5, 10, 5)$:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 4 \\ 2 & 3 & 4 & 5 & 3 & 4 & 5 & 4 & 5 & 5 \\ 5 & 4 & 2 & 3 & 1 & 3 & 4 & 5 & 2 & 1 \\ 2 & 3 & 4 & 5 & 3 & 4 & 5 & 4 & 5 & 5 \\ 1 & 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 4 \end{pmatrix}.$$

When $v \equiv 3 \pmod 4$ is a prime power and $k = v$, there is a general method for constructing designs of the type described in Theorem 4.2. For this case, it is well known (c.f. Raghavarao (1971)) that the quadratic residues $(\operatorname{mod} v)$ form a difference set. Let D be the complement of the quadratic residues in $GF(v)$; hence D is a $(v, (v+1)/2, \lambda)$ difference set. It can be shown that $D' = D - \{0\}$ is a $(v, (v-1)/2, \lambda - 1)$ difference set. In Theorem 4.2 take d_1 to be the $(v-1)/2 \times v$ array with columns $\{D' + x : x \in GF(v)\}$ and $\binom{d_1}{d_0}$ the $(v+1)/2 \times v$ array with columns $\{D + x : x \in GF(v)\}$. Then the array d^* in Theorem 4.2 is optimal in $\mathcal{D}_{tf}(v, v, v)$. (Taking copies of columns, this can be extended to $\mathcal{D}_{tf}(v, b, v)$ with $b \equiv 0 \pmod v$).

Example 4.3. Let $v = k = 7$. For these parameter values, we get the following optimal design in $\mathcal{D}_{tf}(7, 7, 7)$:

$$\begin{pmatrix} 3 & 4 & 5 & 6 & 0 & 1 & 2 \\ 5 & 6 & 0 & 1 & 2 & 3 & 4 \\ 6 & 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 0 & 1 & 2 & 3 & 4 & 5 \\ 5 & 6 & 0 & 1 & 2 & 3 & 4 \\ 3 & 4 & 5 & 6 & 0 & 1 & 2 \end{pmatrix}.$$

For a design d^* of Theorem 4.2,

$$\max_{d \in \mathcal{D}_{tf}(v,b,k)} \operatorname{tr} C_d = \operatorname{tr} C_{d^*} = b(k-2) + (b/k) > b(k-2) = \max_{d \in \mathcal{D}_b(v,b,k)} \operatorname{tr} C_d.$$

Thus, a universally optimal trend-free design is more efficient than a universally optimal binary design of Section 3 when k is odd.

5. Efficiency and Optimal Designs for $k = 3$

To get some idea of the efficiency of designs in Sections 3 and 4, we first determine an upper bound for $\operatorname{tr} C_d$ in $\mathcal{D}(v, b, k)$. Note that for any $d_1 \in \mathcal{D}(v, b, k)$,

$$\operatorname{tr} C_{d_1} < \ b(k-1). \tag{5.1}$$

The inequality in (5.1) is always strict since a binary design cannot be trend-free. Nevertheless, this gives a (conservative) measure of the efficiency of a design d. It follows from (2.5), that $e(d) > \operatorname{tr} C_d / b(k-1)$. If d is a binary design, or d is an optimal trend-free design in $\mathcal{D}_{tf}(v, b, k)$ with k even given by Theorem 4.1, then

$$e(d) > (k-2)/(k-1). \tag{5.2}$$

If d is an optimal trend-free design in $\mathcal{D}_{tf}(v, b, k)$ with k odd given by Theorem 4.2, then

$$e(d) > (k-1)/k. \tag{5.3}$$

For large k it is evident from (5.2) and (5.3) that the optimal designs given in Sections 3 and 4 are highly efficient. When k is small we suspect that (5.2) and (5.3) are overly conservative. For $k = 3$, we have the following theorem:

Theorem 5.1. *For $v \geq k = 3$, the design d^* in Theorem 4.2 is universally optimal in $\mathcal{D}(v, b, 3)$.*

Proof. It can be shown by direct computation that $\operatorname{tr} C_d$ is maximized in $\mathcal{D}(v, b, 3)$ if, for each $j = 1, \ldots, b$, there are two symbols i and $i', i \neq i'$, such that $n_{dij} = 2$ and $n_{di'j} = \delta_{2j}^{i'} = 1$.

In general, however, an optimal trend-free design need not be optimal in $\mathcal{D}(v, b, k)$ as the following example shows.

Example 5.1. For $v = 7$ and $k = 4$ consider two designs in $\mathcal{D}(7, 21, 4)$:

$$d_1 = \begin{pmatrix} 0 & 1 & 3 & 1 & 2 & 4 & 2 & 3 & 5 & 4 & 3 & 6 & 5 & 4 & 0 & 6 & 5 & 1 & 0 & 6 & 2 \\ 3 & 0 & 1 & 4 & 1 & 2 & 5 & 2 & 3 & 3 & 6 & 4 & 4 & 0 & 5 & 5 & 1 & 6 & 6 & 2 & 0 \\ 1 & 3 & 0 & 2 & 4 & 1 & 3 & 5 & 2 & 6 & 4 & 3 & 0 & 5 & 4 & 1 & 6 & 5 & 2 & 0 & 6 \\ 0 & 1 & 3 & 1 & 2 & 4 & 2 & 3 & 5 & 4 & 3 & 6 & 5 & 4 & 0 & 6 & 5 & 1 & 0 & 6 & 2 \end{pmatrix},$$

$$d_2 = \begin{pmatrix} 0 & 0 & 0 & 4 & 5 & 6 & 1 & 1 & 1 & 5 & 6 & 2 & 2 & 5 & 6 & 3 & 3 & 6 & 4 & 6 & 5 \\ 1 & 2 & 3 & 0 & 0 & 0 & 2 & 3 & 4 & 1 & 1 & 3 & 4 & 2 & 2 & 4 & 5 & 3 & 5 & 4 & 6 \\ 1 & 2 & 3 & 0 & 0 & 0 & 2 & 3 & 4 & 1 & 1 & 3 & 4 & 2 & 2 & 4 & 5 & 3 & 5 & 4 & 6 \\ 0 & 0 & 0 & 4 & 5 & 6 & 1 & 1 & 1 & 5 & 6 & 2 & 2 & 5 & 6 & 3 & 3 & 6 & 4 & 6 & 5 \end{pmatrix}.$$

Both C_{d_1} and C_{d_2} are c.s., d_2 is universally optimal in $\mathcal{D}_{tf}(7,21,4)$, but $\operatorname{tr} C_{d_2} = 42 < 50.4 = \operatorname{tr} C_{d_1}$.

Comment. Throughout this paper we have been considering designs which are connected under model (2.1). In general, one can always verify the connectedness of a given design $d \in D(v,b,k)$ by checking to see if C_d has rank $v-1$. There is, to the best of the authors' knowledge, currently no simpler general method available for determining whether or not a given design $d \in D(v,b,k)$ is connected. However, if C_d is c.s., then d is connected unless $C_d = 0$. It is also easy to see that a trend-free design is connected if and only if the corresponding block design is connected. The study of connectedness for other types of designs needs further attention.

Acknowledgement

We are grateful to John Stufken and to the referee for drawing our attention to the literature on semibalanced arrays.

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(Received January 1994; accepted March 1995)