Designs with nearly minimal number of observations and flexible blocking

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Abstract

Consider the class $D(v,B,p,q)$ of connected designs with v treatments and $b \leqslant B$ blocks of size at least p and at most q. Let $D_0(v,B,p,q) \subset D(v,B,p,q)$ be the subclass of designs with the minimum number $n = v+b-1$ of observations needed to estimate the treatment contrasts. It will be shown that, in general, the D-optimal design in $D_0(v,B,p,q)$ with $b=a$ blocks and $v+a-1$ observations has higher D-efficiency than the D-optimal design with $b=a+1$ blocks and $v+a$ observations. Thus, in general, the addition of an extra block parameter cannot be outweighed by the addition of an extra observation. Similar results are shown for A-optimality. For the subclass $D_1(v,B,p,q) \subset D(v,B,p,q)$ of designs having one more than the minimum number of observations, it is shown that the design with fewer blocks is better under the D-criterion unless $(p=2, a=2, v=q+1)$ or $(p=2, a=2, v=3)$ or $(p=2, a=1, v \leqslant q-1)$ or $(p=3, a=1, v=4)$.

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1. Introduction

We consider a situation where up to B blocks are available for an experiment, but not all of these need necessarily be used. For example, in a drug trial, the blocks typically represent subjects, and each subject used in the trial may entail an additional cost, implying that the number of subjects should be kept as small as possible. On the other hand, each subject receives a sequence of drugs throughout the trial, and because of the high dropout rate, it is usually thought advisable to allocate to each subject a sequence no more than three or four drugs depending upon the nature of the trial. Similarly, in industry, each block may represent the use of a machine for a

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certain period of time. The maximum block size would be restricted by the number of observations that can be taken in the time period. Since the use of a machine for an experiment precludes its use in production, the number of blocks would need to be kept small.

Suppose that the number of blocks selected for the experiment is $b \leqslant B$. The jth block is allocated k_j treatments where k_j is some number between the minimum block size p ($p \geqslant 2$) and the maximum block size q ($j = 1, \ldots, b$) inclusive. The total number of observations is fixed at n. We consider very small experiments where n is either fixed to be the minimum possible number of observations $(v+b-1)$ or fixed to be one more than the minimum number $(v+b)$ of observations needed to estimate the treatment contrasts adjusted for blocks. For references and background material on such designs, see Dey et al. (1995). For details on optimality criteria see, for example, Kiefer (1975) or Shah and Sinha (1989).

In this paper, we investigate, in terms of the D- and A-efficiency of the design, whether it is always better to use the smallest number of blocks possible, or whether the addition of an extra block parameter can be outweighed by an extra observation.

Let $D(v, B, p, q)$ be the class of connected designs having v treatments and $b \leqslant B$ blocks with block sizes at least p and at most q. Let n_{ij} denote the number of times that treatment i is observed in block j. We use the standard intra-block model

$$Y_{ijs} = \mu + \beta_j + \tau_i + E_{ijs} \tag{1}$$

where μ is a constant. β_j is the effect of the jth block, and τ_i is the effect of the ith treatment ($i = 1, \ldots, v$; $j = 1, \ldots, b$). If $n_{ij} \geqslant 1$, then Y_{ijs} is the response associated with the sth observation on the ith treatment in the jth block, and E_{ijs} is the corresponding error random variable with mean zero and variance σ^2 ($s = 1, \ldots, n_{ij}$).

For a design $d \in D(v, B, p, q)$ with b ($\leqslant B$) blocks, let C_d be the information matrix for estimating the treatment effects adjusted for block effects under model (1). It is well-known that C_d is given by

$$C_d = R_d - N_d K_d^{-1} N_d',$$

where R_d and K_d are diagonal matrices containing, respectively, the treatment replications $r_{d1}, \ldots, r_{dv}$ and the block sizes $k_{d1}, \ldots, k_{db}$, and where N_d is the incidence matrix with (ij)th element n_{ij}. We denote the eigenvalues of C_d by $\lambda_{d1}, \lambda_{d2}, \ldots, \lambda_{d,(v-1)}, 0$.

In Section 2, we derive inequalities which will be our tools in proving the optimality results. In Section 3, we look at the D-efficiency of designs with the minimum and one more than the minimum number of observations. In the first case, the D-optimal design with fewest blocks is always preferred. In the second case, this is not always true. In particular, when $p = 2$ and the maximum block size is $q = v - 1$, the D-optimal design with 3 blocks is D-better than the D-optimal design with 2 blocks, and when $q \geqslant v + 1$, the D-optimal design with 2 blocks is D-better than the D-optimal design with 1 block. In Section 4, we show that the A-optimal design with fewest blocks is always preferred under the A-criterion in the class of designs with the minimum number of observations.

2. Inequalities

The following theorems will be needed throughout the paper.

Theorem 1. *Let* $q \geqslant k_1 \geqslant k_2 \geqslant \cdots \geqslant k_b \geqslant p$ *be integers satisfying* $\sum_{j=1}^{b} k_j = n$. *Then*

(1) $\prod_{j=1}^{b} k_j \geqslant \prod_{j=1}^{b} k_j^*$, *and*

(2) $\sum_{j=1}^{b} k_j^2 \leqslant \sum_{j=1}^{b} k_j^{*2}$ *where* $k_1^* = k_2^* = \cdots = k_t^* = q$, $k_{t+1}^* = n - t(q-p) - bp + p$, $k_{t+2}^* = \cdots = k_b^* = p$,

$$t = \left[\frac{n-bp}{q-p}\right]^- \tag{2}$$

and $[a]^-$ *denotes the largest integer less than or equal to a.*

Proof. For two integers r and s, where $p \leqslant r \leqslant s \leqslant q$, $rs \geqslant (r-1)(s+1)$ and $r^2+s^2 \leqslant (r-1)^2+(s+1)^2$. Consequently, $\prod_{j=1}^{b} k_j$ is minimized and $\sum_{j=1}^{b} k_j^2$ is maximized when $k_1 = k_2 = \cdots = k_t = q$, $k_{t+1} = \cdots = k_{b-1} = p$ and $k_b = n - tq - (b-t-1)p$, for some integer t. Since $k_b \geqslant p$, where p is the minimum block size, we have $t \leqslant (n-bp)/(q-p)$, and the result follows. □

Theorem 2. *Let* $k_j \geqslant p \geqslant 1$ *and* $x_j \geqslant 0$, $j = 1, \ldots, b$, *be real numbers such that* $\sum_{j=1}^{b} x_j \leqslant p-1$. *Then,*

$$\prod_{j=1}^{b} (k_j + x_j) \leqslant e^{(p-1)/p} \prod_{j=1}^{b} k_j. \tag{3}$$

Proof. We can write,

$$\prod_{j=1}^{b} (k_j + x_j) = \left(\prod_{j=1}^{b} k_j\right)\left(\prod_{j=1}^{b} (1 + x_j/k_j)\right) \leqslant \left(\prod_{j=1}^{b} k_j\right)\left(\prod_{j=1}^{b} (1 + x_j/p)\right)$$

or, since geometric mean is less than or equal to arithmetic mean,

$$\frac{\prod_{j=1}^{b} (k_j + x_j)}{\prod_{j=1}^{b} k_j} \leqslant \prod_{j=1}^{b} (1 + x_j/p) \leqslant \left(1 + \frac{p-1}{pb}\right)^b. \tag{4}$$

Now, $(1 + (p-1)/pb)^b$ is an increasing function in b $(b \geqslant 1)$ and so,

$$\max_{b \geqslant 1} \left(1 + \frac{p-1}{pb}\right)^b = \lim_{b \to \infty} \left(1 + \frac{p-1}{pb}\right)^b = e^{(p-1)/p}. \tag{5}$$

Therefore, from Eqs. (4) and (5), we have,

$$\prod_{j=1}^{b} (k_j + x_j) \Big/ \prod_{j=1}^{b} k_j \leqslant e^{(p-1)/p}. \qquad \square$$

Corollary 1. *Let* $k_j \geqslant p \geqslant 1$ *and* $x_j \geqslant 0$, $j = 1,\ldots,b$, *be real numbers such that* $\sum_{j=1}^{b} x_j \leqslant p-1$. *Then,*

(a) $\prod_{j=1}^{b}(k_j + x_j) \leqslant \alpha \prod_{j=1}^{b} k_j$ *for* $p \leqslant (1-\ln\alpha)^{-1}$, $1 \leqslant \alpha \leqslant \mathrm{e}$

(b) $\prod_{j=1}^{b}(k_j + x_j) \leqslant \mathrm{e} \prod_{j=1}^{b} k_j$ *for* $p < \infty$.

Theorem 3. *Let* $k_j \geqslant p \geqslant 1$ *and* $x_j \geqslant 0$, $j = 1,\ldots,b$, *be real numbers such that* $\sum_{j=1}^{b} x_j \geqslant p-1$. *Then,*

$$\sum_{j=1}^{b}(k_j + x_j)^2 \geqslant 2p(p-1) + \sum_{j=1}^{b} k_j^2. \tag{6}$$

Proof. We note that

$$\sum_{j=1}^{b}(k_j + x_j)^2 = \sum_{j=1}^{b} k_j^2 + 2\sum_{j=1}^{b} k_j x_j + \sum_{j=1}^{b} x_j^2 \geqslant \sum_{j=1}^{b} k_j^2 + 2p\sum_{j=1}^{b} x_j + \sum_{j=1}^{b} x_j^2.$$

Now, since $\min \sum_{j=1}^{b} x_j^2$ such that $\sum_{j=1}^{b} x_j \geqslant p-1$ is when $x_j = (p-1)/b$, $j = 1,\ldots,b$, we have

$$\sum_{j=1}^{b}(k_j + x_j)^2 - \sum_{j=1}^{b} k_j^2 \geqslant 2p(p-1) + \sum_{j=1}^{b} x_j^2 \geqslant 2p(p-1) + (p-1)^2/b. \tag{7}$$

But, $2p(p-1) + (p-1)^2/b$ is a decreasing function in $b\,(b \geqslant 1)$. So,

$$\min_{b \geqslant 1}\{2p(p-1) + (p-1)^2/b\} = \lim_{b\to\infty}\{2p(p-1) + (p-1)^2/b\}$$

$$= 2p(p-1). \tag{8}$$

Therefore, from Eqs. (7) and (8), we have,

$$\sum_{j=1}^{b}(k_j + x_j)^2 - \sum_{j=1}^{b} k_j^2 \geqslant 2p(p-1). \qquad \square$$

Corollary 2. *Let* $k_j \geqslant p \geqslant 1$ *and* $x_j \geqslant 0$, $j = 1,\ldots,b$, *be real numbers such that* $\sum_{j=1}^{b} x_j = p-1$. *Then*

$$\prod_{j=1}^{b}(k_j + x_j) \leqslant \mathrm{e}^{(p-1)/p} \prod_{j=1}^{b} k_j$$

and

$$\sum_{j=1}^{b}(k_j + x_j)^2 \geqslant 2p(p-1) + \sum_{j=1}^{b} k_j^2.$$

3. D-optimality

We can represent a block design d by a bipartite multigraph H_d with two sets of vertices defined by the treatment labels $(T_1, T_2, \ldots, T_v)$ and the block labels $(B_1, B_2, \ldots, B_b)$, (see Harary (1988) for a discussion of bipartite graphs). A pair of vertices (T_i, B_j) is joined by n_{ij} parallel edges, where n_{ij} is defined above. If the design d is connected, the corresponding graph H_d is also connected. The number of spanning trees (i.e. subgraphs having no cycles and covering every vertex) in the graph H_d is called the complexity $c(H_d)$ of the graph. Following the discussion in Dey et al. (1995), it can be shown that

$$\prod_{i=1}^{v-1} \lambda_{di} = vc(H_d) \bigg/ \left[\prod_{j=1}^{b} k_{d_j}\right]. \tag{9}$$

In Section 3.1, we discuss designs with the minimum number of observations, and in Section 3.2, we discuss designs with one more than the minimum number of observations. We note that in the first case, $n = v + b - 1 > \sum_{j=1}^{b} k_{d_j} \geqslant 2b$ so $b \leqslant v - 1$, and in the second case $n = v + b \geqslant 2b$, so that $b \leqslant v$.

3.1. Designs with the minimum number of observations

Let $D_0(v, B, p, q)$ be the subset of designs in $D(v, B, p, q)$ with the minimum number $n = v + b - 1$ of observations needed to estimate the treatment contrasts. Dey et al. (1995) argue that, for any design in this class, the complexity $c(H_d)$ of the associated multigraph is 1. Therefore, from Eq. (9), all designs in $D_0(v, B, p, q)$ with a fixed number b of blocks and a fixed set of block sizes $k_{d1}, \ldots, k_{db}$ are equivalent under D-optimality. Similarly, the design $d^* \in D_0(v, B, p, q)$ that is D-optimal amongst designs with a fixed number b of blocks satisfies

$$\prod_{j=1}^{b} k_{d^*j} = \min_{d \in D_0(v, B, p, q)} \prod_{j=1}^{b} k_{d_j}. \tag{10}$$

Let the number of blocks in design $d \in D_0(v, B, p, q)$ be b_d where $b_{\min} \leqslant b_d \leqslant b_{\max}$. Here, $b_{\max}(b_{\min})$ is the maximum (minimum) number of blocks and is given in Lemma 1.

Lemma 1. *The minimum and maximum number of blocks possible in a design $d \in D_0(v, B, p, q)$ are given by*

$$b_{\min} = \left[\frac{v-1}{q-1}\right]^{+} \quad \text{and} \quad b_{\max} = \min\left(B, \left[\frac{v-1}{p-1}\right]^{-}\right)$$

where $[a]^{+}$ denotes the smallest integer greater than or equal to a.

Proof. The number of observations in a design $d \in D_0(v, B, p, q)$ is $n = v + b_d - 1$, where

$$pb_d \leqslant v + b_d - 1 \leqslant qb_d.$$

Therefore,

$$\frac{v-1}{q-1} \leqslant b_d \leqslant \frac{v-1}{p-1}$$

and, noting that B blocks are available for the experiment, the result follows. □

For b fixed, define

$$\phi(b) = \min_{d \in D_0(v,B,p,q)} \prod_{j=1}^{b} k_{d_j} = \prod_{j=1}^{b} k^*_{d(b)j} = q^{t_b}\, p^{b-t_b-1}[v-1-b(p-1)-t_b(q-p)+p] \tag{11}$$

where

$$t_b = \left[\frac{v-1-b(p-1)}{q-p}\right]^{-}.$$

The RHS of Eq. (11) follows from Theorem 1. Note that by Eq. (9) and the fact that the complexity $c(H_d)$ is 1, D-optimality is equivalent to minimizing $\phi(b)$. In Theorem 4, we show that the D-optimal design with b blocks is D-better than the D-optimal design with $b+1$ blocks, so that the design with fewer blocks is always preferred.

Theorem 4. *Let $\phi(b)$ be defined as in Eq.* (11), *then $\phi(b) < \phi(b+1)$ for $b_{\min} \leqslant b \leqslant b_{\max} - 1$.*

Proof. From Eq. (2) with $n_{b_d} = v + b_d - 1$, we have

$$t_{b_d} = \left[\frac{v-1-b_d(p-1)}{q-p}\right]^{-}.$$

Therefore,

$$t_b = \left[\frac{v-1-b(p-1)}{q-p}\right]^{-} \geqslant \left[\frac{v-1-(b+1)(p-1)}{q-p}\right]^{-} = t_{b+1}. \tag{12}$$

Now, from Eq. (11) and Theorem 1,

$$\phi(b) = \prod_{j=1}^{b} k^*_{d(b)j}$$

where

$$k^*_{d(b)j} = \begin{cases} q, & 1 \leqslant j \leqslant t_b, \\ v-1-b(p-1)-t_b(q-p)+p, & j = t_b+1, \\ p, & t_b+2 \leqslant j \leqslant b. \end{cases} \tag{13}$$

Also,

$$\phi(b+1) = \prod_{j=1}^{b+1} k^*_{d(b+1)j} = p\prod_{j=1}^{b} k^*_{d(b+1)j}$$

where

$$k^*_{d(b+1)j} = \begin{cases} q, & 1 \leqslant j \leqslant t_{b+1}, \\ v-1-(b+1)(p-1)-t_{b+1}(q-p)+p, & j = t_{b+1}+1, \\ p, & t_{b+1}+2 \leqslant j \leqslant b+1. \end{cases} \tag{14}$$

From Eqs. (12)–(14), it is clear that

$$k^*_{d(b)j} \geqslant k^*_{d(b+1)j} \geqslant p, \quad j = 1, \ldots, b. \tag{15}$$

Let $x_j \geqslant 0$, such that

$$k^*_{d(b)j} = k^*_{d(b+1)j} + x_j, \quad j = 1, \ldots, b. \tag{16}$$

Then,

$$\sum_{j=1}^{b} k^*_{d(b)j} = \sum_{j=1}^{b} k^*_{d(b+1)j} + \sum_{j=1}^{b} x_j$$

or

$$\sum_{j=1}^{b} x_j = n_b - (n_{b+1} - p) = p - 1. \tag{17}$$

Now, from Eqs. (13)–(17) and Theorem 2, we have

$$\begin{aligned} \phi(b) = \prod_{j=1}^{b} k^*_{d(b)j} &= \prod_{j=1}^{b} (k^*_{d(b+1)j} + x_j) \\ &\leqslant e^{(p-1)/p} \prod_{j=1}^{b} k^*_{d(b+1)j} \\ &< p \prod_{j=1}^{b} k^*_{d(b+1)j} = \phi(b+1). \qquad \square \end{aligned}$$

Theorems 1 and 4 imply that the D-optimal design in $D_0(v, B, p, q)$ has

$$b = b_{\min} = \left[\frac{v-1}{q-1}\right]^+$$

blocks, where t of these blocks are of maximum size q, and $(b-t-1)$ of the blocks are of minimum size p, and the one remaining block is of size $(v-1)-b(p-1)-t(q-p)+p$ where

$$t = \left[\frac{v-1-b(p-1)}{q-p}\right]^- . \tag{18}$$

Example 1. Let $p=2$, $q=3$, $v=4$, $B=3$, and $n=v+b-1=b+3$. Now $b_{\max}=3$ and $b_{\min}=2$. There are only two non-isomorphic (under treatment permutations) connected designs with $b_{\max}$ blocks, shown as d_1 and d_2 below with blocks as columns. There is only one connected design with $b_{\min}=2$ blocks (upto treatment permutations). This is shown as d_3 below

$$d_1:\ \begin{array}{ccc} 1 & 2 & 3 \\ 2 & 3 & 4 \end{array} \qquad d_2:\ \begin{array}{ccc} 1 & 1 & 1 \\ 2 & 3 & 4 \end{array} \qquad d_3:\ \begin{array}{cc} 1 & 1 \\ 2 & 4 \\ 3 & \end{array}$$

The information matrices of these designs are easily calculated and are not given here. One finds that the non-zero eigenvalues $(\lambda_1, \lambda_2, \lambda_3)$ of these information matrices are (0.2929, 1.0, 1.7071), (0.5, 0.5, 2.0), and (0.4226, 1.0, 1.5774), respectively. $\prod_{i=1}^{3} \lambda_i^{-1}$ is 2.0, 2.0, and 1.5, respectively. Note that the first two designs are equivalent under D-optimality as mentioned in the introduction.

3.2. Designs with one more than the minimal number of observations

Let $D_1(v,B,p,q) \subset D(v,B,p,q)$ be the subclass of connected designs with $b \leqslant B$ blocks and one more than the minimum number of observations needed to estimate the treatment contrasts adjusted for blocks, that is $n=v+b$. Following the proof of Lemma 1 with $n=v+b$, the minimum and maximum possible numbers of blocks in design $d \in D_1(v,B,p,q)$ are, respectively,

$$b_{\min} = \left[\frac{v}{q-1}\right]^{+} \quad \text{and} \quad b_{\max} = \min\left(B, \left[\frac{v}{p-1}\right]^{-}\right).$$

From Eq. (9), the D-optimal design in $D_1(v,B,p,q)$ is the design that minimizes $\prod_{j=1}^{b} k_{dj}$ and maximizes $c(H_d)$. Dey et al. (1995) argue that the complexity $c(H_d)$ of the multigraph H_d for a design $d \in D_1(v,B,p,q)$ is in the range $2 \leqslant c(H_d) \leqslant 2\min(b,v)$. Here $b<v$, so we have $2 \leqslant c(H_d) \leqslant 2b$. Furthermore, when $n=v+b$, for given v,b and block sizes $k_1,\ldots,k_b$ we can always construct a design with $c(H_d)=2b$. For example, we can construct a design with $c(H_d)=2b$, where the b blocks are generated in a cyclic fashion as follows. Block 1 contains treatments 1 to k_1. Block 2 contains treatments k_1 to k_1+k_2-1. Block 3 contains treatments k_1+k_2-1 to $k_1+k_2+k_3-2$. Continue in this manner with the last treatment in block b being treatment 1. Note that the first treatment in any block is the same as the last treatment in the previous block. Obviously permuting treatment labels in the design described above will also yield a design with $c(H_d)=2b$. As a result, we see that the D-optimal design d^* has $c(H_{d^*})=2b$. Consequently, the D-optimal design in $D_1(v,B,p,q)$ with a fixed number b of blocks satisfies Eq. (10) and from Theorem 1 has t_b blocks of size q, $b-t_b-1$ blocks of size p, and one block of size $v-b(p-1)-t_b(q-p)+p$, where t_b is given in Eq. (2) with $n=v+b$, i.e.

$$t_b = \left[\frac{v-b(p-1)}{q-p}\right]^{-}. \tag{19}$$

Define

$$\phi_1(b) = \min_{d\in D_1(v,B,p,q)} \frac{1}{b}\prod_{j=1}^{b} k_{dj} = \frac{1}{b}\prod_{j=1}^{b} k^*_{d(b)j}$$
$$= b^{-1} q^{t_b} p^{b-t_b-1}[v - b(p-1) - t_b(q-p) + p]. \tag{20}$$

A design with complexity $2b$ and which minimizes $\phi_1(b)$ in Eq. (20) is D-optimal, which follows from Eq. (9) and Theorem 1. In Theorem 5, we show that the D-optimal design with b blocks is D-worse than the D-optimal design with $b+1$ blocks when $(p=2, b=2, v=q+1)$ or $(p=2, b=2, v=3)$ or $(p=2, b=1, v\leqslant q-1)$ or $(p=3, b=1, v=4)$. In all other situations, the design with fewer blocks is always preferred.

Theorem 5. *Let $\phi_1(b)$ be defined as in Eq. (20), then $\phi_1(b) > \phi_1(b+1)$ for $(p=2, b=2, v=q+1)$ or $(p=2, b=2, v=3)$ or $(p=2, b=1, v\leqslant q-1)$ or $(p=3, b=1, v=4)$. Otherwise $\phi_1(b) \leqslant \phi_1(b+1)$ for $b_{\min} \leqslant b \leqslant b_{\max}-1$.*

Proof. From Eq. (19) we have

$$t_b = \left[\frac{v-b(p-1)}{q-p}\right]^- \geqslant \left[\frac{v-(b+1)(p-1)}{q-p}\right]^- = t_{b+1}. \tag{21}$$

Also, from Eq. (20) and Theorem 1, we have

$$\phi_1(b) = \frac{1}{b}\prod_{j=1}^{b} k^*_{d(b)j}$$

where

$$k^*_{d(b)j} = \begin{cases} q, & 1\leqslant j\leqslant t_b, \\ v-b(p-1)-t_b(q-p)+p, & j=t_b+1, \\ p, & t_b+2\leqslant j\leqslant b \end{cases} \tag{22}$$

and

$$\phi_1(b+1) = \frac{1}{b+1}\prod_{j=1}^{b+1} k^*_{d(b+1)j} = \frac{p}{b+1}\prod_{j=1}^{b} k^*_{d(b+1)j}$$

where

$$k^*_{d(b+1)j} = \begin{cases} q, & 1\leqslant j\leqslant t_{b+1}, \\ v-(b+1)(p-1)-t_{b+1}(q-p)+p, & j=t_{b+1}+1, \\ p, & t_{b+1}+2\leqslant j\leqslant b+1. \end{cases} \tag{23}$$

From Eqs. (21)–(23) it follows that

$$k^*_{d(b)j} \geqslant k^*_{d(b+1)j} \geqslant p, \quad j=1,\ldots,b. \tag{24}$$

Let $x_j \geqslant 0$, such that

$$k^*_{d(b)j} = k^*_{d(b+1)j} + x_j, \quad j = 1, \ldots, b. \tag{25}$$

Then,

$$\sum_{j=1}^{b} k^*_{d(b)j} = \sum_{j=1}^{b} k^*_{d(b+1)j} + \sum_{j=1}^{b} x_j$$

or

$$v + b = (v + b + 1) - p + \sum_{j=1}^{b} x_j$$

or

$$\sum_{j=1}^{b} x_j = p - 1. \tag{26}$$

Therefore, from Eqs. (22)–(26) and Theorem 2, we have

$$\begin{aligned}\phi_1(b) = \frac{1}{b}\prod_{j=1}^{b} k^*_{d(b)j} &= \frac{1}{b}\prod_{j=1}^{b} (k^*_{d(b+1)j} + x_j) \\ &\leqslant \frac{1}{b} e^{(p-1)/p} \prod_{j=1}^{b} k^*_{d(b+1)j} \\ &= \frac{b+1}{bp} e^{(p-1)/p} \phi_1(b+1).\end{aligned} \tag{27}$$

Now, define $E = \phi_1(b)/\phi_1(b+1)$. Then Eq. (27) implies

$$E \leqslant \frac{b+1}{bp} e^{(p-1)/p}. \tag{28}$$

We consider the following exhaustive cases separately.

(1) $p \geqslant 3$, $b \geqslant 2$,
(2) $p \geqslant 5$, $b = 1$,
(3) $p = 2$, $b \geqslant 5$,
(4) $p = 2$, $b = 3$ or 4,
(5) $p = 2$, $b = 2$,
(6) $p = 2$ or 3 or 4, $b = 1$.

Case 1: $p \geqslant 3$, $b \geqslant 2$. We obtain from Eq. (27)

$$\frac{\phi_1(b)}{\phi_1(b+1)} \leqslant \frac{(b+1)}{bp} e^{(p-1)/p} \leqslant \max_{b \geqslant 2, p \geqslant 3} \left\{ \frac{(b+1)}{bp} e^{(p-1)/p} \right\} = \frac{3e^{2/3}}{2 \times 3} < 0.98$$

i.e., $\phi_1(b) < \phi_1(b+1)$.

Case 2: $p \geqslant 5$, $b = 1$. For $b = 1$, from Eq. (27) we have

$$\frac{\phi_1(b)}{\phi_1(b+1)} \leqslant \frac{(b+1)}{bp} e^{(p-1)/p} = \frac{2e^{(p-1)/p}}{p} \leqslant \max_{p \geqslant 5} \left\{ \frac{2e^{(p-1)/p}}{p} \right\} = \frac{2e^{4/5}}{5} < 0.90$$

i.e., $\phi_1(b) < \phi_1(b+1)$.

Case 3: $p=2$, $b\geqslant 5$. For $p=2$, from Eq. (27) we have

$$\frac{\phi_1(b)}{\phi_1(b+1)} \leqslant \frac{(b+1)}{bp} e^{(p-1)/p} = \frac{(b+1)}{2b} e^{1/2} \leqslant \max_{b\geqslant 5} \left\{ \frac{(b+1)}{2b} e^{1/2} \right\} = \frac{6e^{1/2}}{2\times 5} < 0.99$$

i.e., $\phi_1(b) < \phi_1(b+1)$.

Case 4: $p=2$, $b=3$ or 4. For simplicity of notation here and below, let $k=k^*_{d(b+1)b_{+1}+1}$. For $p=2$ and $k\geqslant 2$, from Eqs. (19), (20), (22) and (24), one can show

$$\frac{\phi_1(b)}{\phi_1(b+1)} = \frac{(k+1)/b}{2k/(b+1)} \leqslant \max_{\substack{k\geqslant 2\\ b=3 \text{ or } 4}} \left\{ \frac{(k+1)/b}{2k/(b+1)} \right\}$$
$$= \max_{\substack{k\geqslant 2\\ b=3 \text{ or } 4}} \left\{ \frac{(k+1)}{2k} \frac{(b+1)}{b} \right\} = \frac{3\times 4}{2\times 2\times 3} = 1.$$

Case 5: $p=2$, $b=2$

$$\frac{\phi_1(b)}{\phi_1(b+1)} = \frac{(k+1)/2}{2k/3} = \frac{3(k+1)}{4k}.$$

Now, $\phi_1(b)/\phi_1(b+1) \leqslant 1$ if $3(k+1)/4k \leqslant 1$ or if $k\geqslant 3$.

This is true unless $d(b+1)$ has one block of size q and two blocks of size 2 (which implies that $q+4=v+3$, i.e. $q=v-1$) or unless $d(b+1)$ has three blocks of size 2 (which implies that $v=3$ and $q\geqslant 3$). Such designs for $v=3$ are,

$d(b+1)$: 1 2 3 $\qquad \phi_1(b+1) = \frac{1}{3}\times 2^3 = 2.67$
2 3 1

$d(b)$: 1 3 $\qquad \phi_1(b) = \frac{1}{2}\times 3\times 2 = 3.0$
2 1
3

Case 6: $p=4$ *or* 3 *or* 2, $b=1$. In this case, we have $\phi_1(2)=\frac{1}{2}pk$ (resulting from two blocks of sizes p and k) and $\phi_1(1)=k+p-1$ (resulting from one block of size $k+p-1$). Hence

$$E = \frac{\phi_1(b)}{\phi_1(b+1)} = \frac{2(k+p-1)}{pk}.$$

For $p=4$, $E=2(k+3)/4k=(k+3)/2k$. Now, $E\leqslant 1$ if $(k+3)/2k\leqslant 1$ or if $k\geqslant 3$ which is true.

For $p=3$,

$$E = \frac{2(k+2)}{3k}\frac{2(v+1)}{3(v-1)} \leqslant 1.$$

Now, $E\leqslant 1$ if $2(k+2)/3k\leqslant 1$ or if $k\geqslant 4$.

This is true unless $d(b+1)$ has two blocks of size 3 and $d(b)$ has one block of size 5 (which implies that $v=4$ and $q \geqslant 5$). Such designs are,

$$d(b+1):\ \begin{matrix} 1 & 3 \\ 2 & 4 \\ 3 & 1 \end{matrix} \qquad \phi_1(b+1)=\tfrac{1}{2}\times 3^2=4.5$$

$$d(b):\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 4 \end{matrix} \qquad \phi_1(b)=\tfrac{1}{1}\times 5=5.0$$

For $p=2$, $E=2(k+1)/2k=(k+1)/k$. Now $E>1$.

Here $d(b+1)$ has one block of size v and one block of size 2, and $d(b)$ has one block of size $v+1$, i.e., $q \geqslant v+1$.

Example 2. Let $p=2$, $q=5$, and $v=4$. Then $b_{\max}=4$ and $b_{\min}=1$. Here $q=v+1$ and, therefore, we expect the D-optimal design with 2 blocks to be D-better than that with 1 block. D-optimal designs with 2 and 1 blocks, have $\phi_1(2)=\frac{1}{2}\times 4\times 2=4.0$ and $\phi_1(1)=\frac{1}{1}\times 5=5.0$, respectively. Thus the D-optimal design has two blocks and is

$$d(2):\ \begin{matrix} 1 & 4 \\ 2 & 1 \\ 3 & \\ 4 & \end{matrix}$$

4. A-optimality

Since the form of A-optimal designs with one more than the minimum number of observations and unequal block sizes ($k_j \geqslant 2$) is, at present, unknown, we only consider the class of designs $D_0(v,B,p,q) \subset D(v,B,p,q)$ with the minimum number of observations. We wish to determine an A-optimal design in this class. For each possible value of b and set of block sizes $k_1,\ldots,k_b$, it can be shown that an A-optimal design is the design $d(b;k_1,\ldots,k_b)$ in which a particular treatment, say treatment 1, is allocated once to each block, and the remaining $v-1$ treatments are each allocated to one of the remaining $\Sigma(k_j-1)$ experimental units. (The proof follows the lines of the proof of the corresponding theorem for equal block sizes given by Mandal et al. (1991)).

Lemma 2. *For a design $d(b; k_1,\dots,k_b)$ defined above, the average variance of the least squares estimators of the pairwise comparisons $\tau_i - \tau_j$ is*

$$V = \frac{2}{v(v-1)}\left[(2v+1)(v-1) + b - \sum_{j=1}^{b} k_j^2\right]\sigma^2. \tag{29}$$

Proof. It is straightforward to show that the least squares estimators of the pairwise comparisons $\tau_i - \tau_j$ have variances

$$\mathrm{Var}(\hat{\tau}_i - \hat{\tau}_j) = \begin{cases} 2\sigma^2, & i=1,\ j=2,\dots,v, \\ 2\sigma^2, & \text{if } i \text{ and } j \text{ are in the same block, } 2 \leqslant i < j \leqslant v, \\ 4\sigma^2, & \text{if } i \text{ and } j \text{ are in different blocks, } 2 \leqslant i < j \leqslant v. \end{cases}$$

Consequently, the average variance of the pairwise comparison estimators for design d is

$$V(d) = \frac{2}{v(v-1)}\left[2(v-1) + 2\sum_{j=1}^{b}\binom{k_j-1}{2}\right.$$

$$\left. + 4\left(\binom{v}{2} - (v-1) - \sum_j \binom{k_j-1}{2}\right)\right]\sigma^2$$

$$= \frac{2}{v(v-1)}\left[-2(v-1) - 2\sum_{j=1}^{b}\binom{k_j-1}{2} + 4\binom{v}{2}\right]\sigma^2$$

$$= \frac{2}{v(v-1)}\left[2(v-1)^2 - \sum_{j=1}^{b}(k_j-1)(k_j-2)\right]\sigma^2$$

$$= \frac{2}{v(v-1)}\left[(2v+1)(v-1) + b - \sum_{j=1}^{b} k_j^2\right]\sigma^2$$

as required. □

By virtue of Lemma 2, an A-optimal design in $D_0(v,B,p,q)$, amongst designs with a fixed number b of blocks, is the design d for which $\sum_{j=1}^{b} k_{d_j}^2$ is a maximum and $\sum_{j=1}^{b} k_{d_j} = v + b - 1$. Thus, from Theorem 1, an A-optimal design with b blocks has

t_b blocks of maximum size q, one block of size $(v-1)-b(p-1)-t_b(q-p)+p$, and $(b-t_b-1)$ blocks of minimum size p, where $t_b=[(v-1-b(p-1))/(q-p)]^-$.

For b fixed, define $\phi_2(b)$ to be

$$\phi_2(b)=\max_{d\in D_0(v,B,p,q)}\left(b-\sum_{j=1}^{b}k_{d_j}^2\right)=b-\sum_{j=1}^{b}k_{d(b)_j}^{*^2}$$

$$=b-t_bq^2-(b-t_b-1)p^2-[(v-1)-b(p-1)-t_b(q-p)+p]^2. \tag{30}$$

In Theorem 6, we show that $\phi_2(b)<\phi_2(b+1)$ for $b_{\min}\leqslant b\leqslant b_{\max}-1$, with

$$b_{\max}=\min\left(B,\left[\frac{v-1}{p-1}\right]^-\right)\quad\text{and}\quad b_{\min}=\left[\frac{v-1}{q-1}\right]^+.$$

Thus, under the A-optimality criterion, an A-optimal design with fewer blocks is always preferred in the class of designs with $n=v+b-1$ observations.

Theorem 6. *Let $\phi_2(b)$ be defined as in Eq.* (30), *then $\phi_2(b)<\phi_2(b+1)$ for $b_{\min}\leqslant b\leqslant b_{\max}-1$.*

Proof. From Eq. (30) and Theorem 1, we have

$$\phi_2(b)=b-\sum_{j=1}^{b}k_{d(b)j}^{*^2} \tag{31}$$

where $k^*_{d(b)j}$, $j=1,\dots,b$, are as in Eq. (13), and

$$\phi_2(b+1)=b+1-\sum k_{d(b+1)j}^{*^2}=b+1-p^2-\sum_{j=1}^{b}k_{d(b+1)j}^{*^2} \tag{32}$$

where $k^*_{d(b+1)j}$, $j=1,\dots,b$ are as in Eq. (14). Now by the same argument as in Theorem 4 and using Theorem 3, we have

$$\phi_2(b)=b-\sum_{j=1}^{b}k_{d(b)j}^{*^2}$$

$$=b-\sum_{j=1}^{b}(k^*_{d(b+1)j}+x_j)^2$$

$$\leqslant b-2p(p-1)-\sum_{j=1}^{b}k_{d(b+1)j}^{*^2}$$

$$=\phi_2(b+1)-(p-1)^2<\phi_2(b+1). \qquad \square$$

Theorems 1 and 6 imply that an A-optimal design in $D_0(v, B, p, q)$, is the design $d^*(b; k_1, \ldots, k_b)$ with $b = b_{\min}$ blocks, where t of these blocks are of maximum size q, and $(b - t - 1)$ of the blocks are of minimum size p, and the one remaining block is of size $(v - 1) - b(p - 1) - t(q - p) + p$, where t is given in Eq. (18). Note this is also the D-optimal design when $n = v + b - 1$.

In the next example, inverses are assumed to be Moore–Penrose inverses.

Example 3. Consider the three designs d_1, d_2 and d_3 from Example 1. The design d_1 does not belong to the subclass of A-optimal designs with $b = 3$ blocks. Since trace $C^- = \sum_{i=1}^{3} \lambda_i^{-1}$, it can be verified that

$$\operatorname{trace} C_1^- = 5.0, \quad \operatorname{trace} C_2^- = 4.5, \quad \operatorname{trace} C_3^- = 4.0.$$

Now d_2 is an A-optimal design with $b = 3$ blocks and d_3 is an A-optimal design with $b = 2$ blocks in $D_0(4, 3, 2, 3)$. Consequently, the design with $b = 2 = b_{\min}$ blocks is A-optimal in $D_0(4, 3, 2, 3)$.

An alternative calculation for trace C_2^- and trace C_3^- uses Eq. (29) since, for an A-optimal design, $V = 2(v - 1)^{-1} \operatorname{trace} C^-$. Thus, we have

$$\begin{aligned} d_2\text{: } \operatorname{trace} C_2^- &= v^{-1}\left[(2v + 1)(v - 1) + b - \sum_{j=1}^{b} k_j^2\right] \\ &= 4^{-1}[(9)(3) + 3 - (4 + 4 + 4)] = 4.5 \\ d_3\text{: } \operatorname{trace} C_3^- &= 4^{-1}[(9)(3) + 2 - (9 + 4)] = 4.0. \end{aligned}$$

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