D-optimal designs with minimal and nearly minimal number of units

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Abstract

D-optimal designs are identified in classes of connected block designs with fixed block size when the number of experimental units is one or two more than the minimal number required for the design to be connected. An application of one of these results is made to identify D-optimal designs in a class of minimally connected row–column designs. Graph-theoretic methods are employed to arrive at the optimality results.

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1. Introduction

Suppose it is desired to investigate the effect of $v(\geqslant 2)$ treatments using a block design d, having b blocks each of size $k(\geqslant 2)$. For a given block design d with parameters v, b, k, let $N_d = (n_{dij})$ be the $v \times b$ incidence matrix, where n_{dij} is the number of times the ith treatment appears in the jth block of d, $i = 1, 2, \ldots, v$, $j = 1, 2, \ldots, b$. Under the standard homoscedastic fixed effects model, the coefficient matrix of the reduced normal equations for estimating linear functions of treatment effects, using d, is

$$C_d = R_d - k^{-1} N_d N_d', \tag{1.1}$$

where

$$R_d = \mathrm{diag}(r_{d1}, r_{d2}, \ldots, r_{dv}) \quad \text{and} \quad r_{di} = \sum_{j=1}^{b} n_{dij}.$$

It is well known that all treatment contrasts are estimable using d if and only if d is *connected*, or, equivalently, if and only if $\text{Rank}(C_d) = v - 1$. A necessary condition for a block design d to be connected is that

$$bk \geqslant b + v - 1 = n_0 \text{ (say)}. \tag{1.2}$$

In the recent past, several papers have appeared in the literature which deal with the optimality of *block* designs when the number of experimental units is small, typically n_0 or $(n_0 + 1)$ (Mukerjee et al., 1986; Krafft, 1990; Mukerjee and Sinha, 1990; Bapat and Dey, 1991; Mandal et al., 1991; Birkes and Dodge, 1991). For $i = 0, 1, 2$, let $\mathscr{D}_i(v, b, k)$, respectively, denote the class of all connected block designs with v treatments, b blocks and constant block size k, satisfying

$$bk = b + v + i - 1. \tag{1.3}$$

Also, let $\mathscr{D}^*(v, b, n)$ denote the class of all connected block designs with v treatments, b blocks and n experimental units (block sizes being arbitrary). Mukerjee et al. (1986) and Krafft (1990) independently proved that all designs in $\mathscr{D}^*(v, b, n_0)$ are equivalent according to the D-optimality criterion for the joint estimation of treatment and block contrasts (For a description of the various optimality criteria, see, e.g. Shah and Sinha. 1989). Mukerjee and Sinha (1990) and Birkes and Dodge (1991) obtained optimal designs in $\mathscr{D}^*(v, b, n_0 + 1)$, the former with respect to the D-criterion and the latter with respect to A- and a modified E-criterion. Both these papers relate to the problem of joint estimation of treatment and block contrasts. For the problem of inferring on treatment contrasts alone, A-, D- and E-optimality of designs in $\mathscr{D}_0(v, b, k)$ has been studied by Bapat and Dey (1991) and Mandal et al. (1991).

The purpose of this communication is to present additional optimality results for designs in $\mathscr{D}_1(v, b, k)$ and $\mathscr{D}_2(v, b, k)$. The optimality criterion chosen is the D-optimality criterion. We use a graph-theoretic formulation of the D-criterion to derive results on block designs, following essentially Gaffke (1982). These results are given in Sections 2 and 3.

In the context of connected row–column designs with minimal or near minimal number of experimental units, optimality results are hitherto largely unknown. Chatterjee and Mukerjee (1993) have recently obtained results on D-optimality of minimally connected three-factor designs in which one of the factors has just two levels. In Section 4, we identify D-optimal designs in the class of minimally connected row–column designs with two rows, using the results of Section 2. Throughout the paper, we consider the problem of inferring on treatment contrasts alone.

2. D-optimal block designs in $\mathscr{D}_1(v, b, k)$

Suppose $\mathscr{D}(v, b, k)$ is the class of all connected block designs with v treatments, b blocks and (constant) block size $k \geqslant 2$, and let $d \in \mathscr{D}(v, b, k)$. Let the eigenvalues of

C_d be $0 = \lambda_{d0} < \lambda_{d1} \leqslant \lambda_{d2} \leqslant \cdots \leqslant \lambda_{d,v-1}$. A design $d^* \in \mathscr{D}(v,b,k)$ is D-optimal over $\mathscr{D}(v,b,k)$ if and only if

$$\prod_{i=1}^{v-1} \lambda_{d^*i} = \max_{d \in \mathscr{D}} \prod_{i=1}^{v-1} \lambda_{di}, \tag{2.1}$$

where, for $i = 1,2,\ldots,v-1$, $\{\lambda_{d^*i}\}$ are the positive eigenvalues of C_{d^*}.

It is known that for an arbitrary connected block design, d, C_d has all its cofactors equal and positive, and,

$$\prod_{i=1}^{v-1} \lambda_{di} = v\,Co(C_d) \tag{2.2}$$

where $Co(C_d)$ is the common cofactor of C_d.

A block design d with v treatments, b blocks and block size k can be described by a bipartite multigraph H_d with treatment labels $1,2,\ldots,v$ and block labels $\beta_1,\beta_2,\ldots,\beta_b$ as its vertices. A pair of vertices (i,β_j) is joined by n_{dij} parallel edges. A block design d is connected if and only if the corresponding multigraph H_d is connected in the graph-theoretic sense. It has been shown by Gaffke (1982) that for such a connected block design d,

$$\prod_{i=1}^{v-1} \lambda_{di} = (v/k^b)c(H_d) \tag{2.3}$$

where, $c(H_d)$ is the number of *spanning trees* in the bipartite graph H_d.

Thus, we infer that a design d^* is D-optimal over $\mathscr{D}(v,b,k)$ if and only if it maximizes $c(H_d)$ over $\mathscr{D}$, or equivalently, if and only if, d^* is such that H_{d^*} has the maximal number of spanning trees. We use the above formulation to obtain D-optimal block design in $\mathscr{D}_1(v,b,k)$ and $\mathscr{D}_2(v,b,k)$.

Recall that for any arbitrary $d \in \mathscr{D}_1(v,b,k)$,

$$bk = b + v. \tag{2.4}$$

It was shown by Bapat and Dey (1991) that for any $d \in \mathscr{D}_0(v,b,k)$, H_d is a tree itself and hence has precisely one spanning tree. The bipartite graph associated with any design in $\mathscr{D}_1(v,b,k)$ has precisely one more edge than the number of edges in the bipartite graph of a design in $\mathscr{D}_0(v,b,k)$. The consequence of adding one more edge to a tree (recall that the bipartite graph of a design in $\mathscr{D}_0(v,b,k)$ is a tree) is that now we have precisely one cycle, *provided* the extra edge is not a multiple edge. But, if there is a multiple edge, the number of spanning trees is exactly two. Note that the bipartite graph will have a multiple edge if and only if the design is nonbinary. Since the length of a cycle is at least three and the number of spanning trees is precisely the length of the cycle, it follows that a non binary block design cannot be D-optimal in $\mathscr{D}_1(v,b,k)$. We can therefore restrict the search for a D-optimal design in $\mathscr{D}_1(v,b,k)$ to the class of binary designs, giving rise to graphs with exactly one cycle.

Since the graph is bipartite, the length of the cycle cannot exceed $2\min(b,v) = 2b$, by virtue of (2.4). Hence, we have

Lemma 1. *For any $d \in \mathscr{D}_1(v,b,k)$,*

$$c(H_d) \leqslant 2b. \tag{2.5}$$

In view of Lemma 1, if there is a $d^* \in \mathscr{D}_1(v,b,k)$ such that $c(H_{d^*}) = 2b$, then d^* is D-optimal in $\mathscr{D}_1(v,b,k)$. Suppose d^* is a design given below with rows as blocks:

$$d^* = \begin{matrix} 1 & 2 & \ldots & k-1 & k \\ k & k+1 & \ldots & 2k-2 & 2k-1 \\ 2k-1 & 2k & \ldots & 3k-3 & 3k-2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (b-2)(k-1)+1 & (b-2)(k-1)+2 & \ldots & (b-1)(k-1) & (b-1)(k-1)+1 \\ (b-1)(k-1)+1 & (b-1)(k-1)+2 & \ldots & b(k-1) & 1 \end{matrix} \tag{2.6}$$

We claim that d^* given by (2.6) is D-optimal in $\mathscr{D}_1(v,b,k)$. Clearly, $d^* \in \mathscr{D}_1(v,b,k)$. The graph H_{d^*} has precisely one cycle, given by

$$\begin{aligned}&(1,B_1),(B_1,k),(k,B_2),(B_2,2k-1),(2k-1,B_3),(B_3,3k-2),\ldots,\\ &((b-2)(k-1)+1,B_{b-1}),(B_{b-1},(b-1)(k-1)+1),\\ &((b-1)(k-1)+1,B_b),(B_b,1).\end{aligned}$$

The length of this cycle is clearly $2b$ and hence

$$c(H_{d^*}) = 2b.$$

Observe that a bipartite graph with a unique cycle of length $2b$ and with no multiple edges is isomorphic to the graph of the design d^*. Hence the design d^* is *uniquely* D-optimal in $\mathscr{D}_1(v,b,k)$ (upto isomorphism). Summarizing, we therefore have

Theorem 1. *The design d^* in (2.6) is uniquely D-optimal in $\mathscr{D}_1(v,b,k)$ for all $k \geqslant 2$.*

3. D-optimal block designs in $\mathscr{D}_2(v,b,k)$

For an arbitrary block design $d \in \mathscr{D}_2(v,b,k)$,

$$bk = b + v - 1. \tag{3.1}$$

To begin with, we assume that $k \geqslant 3$. Let H_d be the bipartite graph associated with a block design $d \in \mathscr{D}_2(v,b,k)$. Then the number of edges in H_d is two more than that in a graph of a design in $\mathscr{D}_0(v,b,k)$. This leads to the following four posibilities:

H_d has either

(i) no cycles (only multiple edges); or

(ii) one cycle and a multiple edge; or

(iii) two vertex-disjoint cycles; or

(iv) three cycles.

The number of spanning trees in each of the above possibilities are as under:

(i) at most four;

(ii) at most $4(b-1)$;

(iii) at most $b_1 b_2$, where b_1 and b_2 are the cycle lengths of the two cycles, $b_1 + b_2 \leqslant 2b$;

(iv) $xy + yz + zx$, where the lengths of the three cycles are $x+y, y+z$ and $z+x$, $x+y \leqslant 2b, y+z \leqslant 2b, z+x \leqslant 2b, x+y+z \leqslant 2b+2$ and $x+y, y+z, z+x$ are all even integers. The last inequality in (iv) above is established by counting the vertices in H_d that are block labels of d.

It is not difficult to see that for $b \geqslant 3$, the maximum number of spanning trees arises in case (iv) only. Therefore, in order to obtain a D-optimal design in $\mathscr{D}_2(v,b,k)$, one has to first solve the following problem:-

$$\begin{aligned} &\text{maximize} && S = xy + yz + zx \\ &\text{subject to} && x+y \leqslant 2b, \quad y+z \leqslant 2b, \quad z+x \leqslant 2b, \\ &&& x+y+z \leqslant 2b+2, \quad x+y, \quad y+z, \quad z+x \\ &&& \text{being all even integers.} \end{aligned} \tag{3.2}$$

We attack this problem by considering several cases.

Case (a): $(2b+2)/3$ is an integer.

Clearly in this case, $x = y = z = (2b+2)/3$ is the solution for the problem (3.2), and with these values of x, y, z, the maximum number of spanning trees is $4(b+1)^2/3$.

The next question is: Does there exist a design satisfying the above values of x, y and z? We answer this question in the affirmative later in this section.

Case (b): $(2b+2)/3 = n + \frac{1}{3}$, n being an integer.

We take $x+y+z = 2b+2$ in this case, as it can be shown that the maximum of $S = xy + yz + zx$ when $x+y+z < 2b+2$ is strictly smaller than the maximum of S when $x+y+z = 2b+2$. In view of the other conditions on x, y, z in (3.2), we must have each of x, y and z an even integer.

Since $2b+2 = 3n+1$, n must be an odd integer, say $n = 2m-1$. A solution to (3.2) is then $x = 2m+2 = y, z = 2m$, and with these values of x, y and z, the maximum number of spanning trees is $4b(b+2)/3$. There indeed is a design for which these values of x, y, z are attained. We discuss this design later in this section.

Case (c): $(2b+2)/3 = n + \frac{2}{3}$, n an integer.

In this case, since $2b+2 = 3n+2$, n must be an even integer, say $n = 2m$. A solution to (3.2) in this case is given by $x = 2m = y$, $z = 2m+2$. The maximum number of spanning trees is then $4(b^2+2b)/3$.

We now describe a design giving rise to the maximum number of spanning trees in each of the three cases considered above. Since we have already determined the values of x, y and z giving rise to the maximum number of spanning trees in the three cases (a), (b) and (c), we simply show how these values of x, y and z can actually be achieved. Let d^{**} be a design constructed as follows: Suppose the blocks of d^{**} are $B_1, B_2, \ldots, B_b$ and treatment labels $1, 2, \ldots, v$. Initially, we put in B_1 the treatments $1, (x+z)/2, (2x+z)/2$ and in block $B_{(z+2)/2}$, the treatments $z/2, z/2+1, (z+x)/2+1$. For $i = 2, 3, \ldots, (z+x)/2$, $i \neq (z+2)/2$, in B_i, we put the treatments $i-1, i$. Finally, for $j = (z+x)/2+1, \ldots, b$, in B_j we put treatments $j, j+1$. The remaining treatments are arbitrarily allocated to all these blocks so as to make each a binary block of size k. It can be verified that in the graph of the design d^{**}, there are three cycles of lengths $x+y$, $y+z$, $z+x$. Note that in all the three cases, $y = x$. It can be seen that any graph with precisely three cycles of lengths $x+y$, $y+z$, $z+x$ is isomorphic to the graph of the design d^{**}. We thus have

Theorem 2. *The design d^{**} constructed above is uniquely (upto isomorphism) D-optimal in $\mathscr{D}_2(v,b,k)$, for all $b \geqslant 3, k \geqslant 3$.*

For $b = 2$, the design with the following blocks can be verified to be D-optimal in $\mathscr{D}_2(v,2,k)$:

$$d^{**} = \begin{matrix} (1 & 2 & 3 & \ldots & k-1 & k) \\ (k-1 & k & k+1 & \ldots & v & 1). \end{matrix}$$

For $k = 2$, clearly the above construction procedure does not work. However, proceeding on lines similar to the case $k \geqslant 3$, one can show that the design with the following block contents is D-optimal in $\mathscr{D}_2(v,b,2)$:

$$(1,2);(2,3);(3,4);\ldots;((z+x)/2,1);(z/2+1,(z+x)/2+1);$$
$$((z+x)/2+1,(z+x)/2+2);((z+x)/2+2,(z+x)/2+3);\ldots;(v,1),$$

where (i) $x = y = z = 2b/3$, if $2b/3$ is an integer, (ii) $x = y = n+1, z = n-1$, if $2b = 3n+1$, (iii) $x = y = n, z = n+2$, if $2b = 3n+2$. Note that for $k = 2$, $x+y+z = 2b$ and that we must have $b \geqslant 3$.

4. D-optimal row–column designs with minimal number of units

Suppose v treatments are to be tested via a row column design d_{RC} with k rows and b columns. A necessary condition for a row–column design d_{RC} to be connected is that

$$bk \geqslant b+v+k-2. \tag{4.1}$$

We consider designs with $k = 2$. For this special case, (4.1) reduces to

$$b \geqslant v. \tag{4.2}$$

Therefore, a necessary condition for a row column design with $k = 2$ rows to be *minimally connected* is that

$$b = v. \tag{4.3}$$

Let $\bar{\mathscr{D}}(v, b, k)$ be the class of all connected row-column designs with v treatments, b columns and k rows. The coefficient matrix of the reduced normal equations for treatment effects, using a design $d_{\mathrm{RC}} \in \bar{\mathscr{D}}(v, b, k)$ is

$$\bar{C}_{d_{\mathrm{RC}}} = \boldsymbol{R}_{d_{\mathrm{RC}}} - \boldsymbol{N}_1\boldsymbol{N}_1'/k - b^{-1}\boldsymbol{N}_2(\boldsymbol{I}_k - \boldsymbol{J}_k/k)\boldsymbol{N}_2', \tag{4.4}$$

where $\boldsymbol{N}_1$ (respectively $\boldsymbol{N}_2$) is the treatment vs column (respectively row) incidence matrix of d_{RC}, $\boldsymbol{R}_{d_{\mathrm{RC}}}$ is the diagonal matrix of treatment replications in the design d_{RC} and $\boldsymbol{J}_k$ is a $k \times k$ matrix of all ones. We can rewrite (4.4) as

$$\bar{\boldsymbol{C}}_{d_{\mathrm{RC}}} = \boldsymbol{C}_d^* - b^{-1}\boldsymbol{N}_2(\boldsymbol{I}_k - \boldsymbol{J}_k/k)\boldsymbol{N}_2' \tag{4.5}$$

where

$$\boldsymbol{C}_d^* = \boldsymbol{R}_{d_{\mathrm{RC}}} - \boldsymbol{N}_1\boldsymbol{N}_1'/k \tag{4.6}$$

is the $\boldsymbol{C}$-matrix of a block design obtained by treating the columns of d_{RC} as blocks.

Now, from (4.5), it is clear that $\bar{\boldsymbol{C}}_{d_{\mathrm{RC}}} \leqslant \boldsymbol{C}_d^*$, where for a pair of nonnegative definite matrices A and B, $A \geqslant B$ indicates that $A - B$ is nonnegative definite. It follows that

$$Co(\bar{\boldsymbol{C}}_{d_{\mathrm{RC}}}) \leqslant Co(\boldsymbol{C}_d^*) \leqslant \max Co(\boldsymbol{C}_d^*). \tag{4.7}$$

Consider a row–column design $d_{\mathrm{RC}}^* \in \bar{\mathscr{D}}(v, v, 2)$ given by

$$d_{\mathrm{RC}}^* = \begin{pmatrix} 1 & 2 & 3 & \cdots & v-1 & v \\ 2 & 3 & 4 & \cdots & v & 1 \end{pmatrix}. \tag{4.8}$$

It is easy to verify that for the design (4.8), one has equality in the first inequality in (4.7) and by Theorem 1, in the second one. Hence we have

Theorem 3. *The design d_{RC}^* in (4.8) is* D-*optimal in $\bar{\mathscr{D}}(v, v, 2)$.*

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