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ON THE E-OPTIMALITY OF PBIB DESIGNS WITH A SMALL NUMBER OF BLOCKS[1]

BY GREGORY M. CONSTANTINE

Indiana University

It is shown that several families of PBIB designs with relatively few blocks are E-optimal over the collection of all block designs. Among these are: the Partial Geometries with two associate classes; PBIB designs with $\lambda_1 = 1$, $\lambda_2 = 0$ and fewer blocks than varieties; PBIB designs with triangular schemes of size n, $\lambda_1 = 0$, $\lambda_2 = 1$ and block size $k \geq n/2$ (or $\lambda_1 = 1$, $\lambda_2 = 0$ and $k \geq n - 1$); PBIB designs with L_i schemes based on v varieties with $\lambda_1 = 0$, $\lambda_2 = 1$, $k \geq \sqrt{v}$ (or $\lambda_1 = 1$, $\lambda_2 = 0$ and either $i - 1 \leq \sqrt{v} \leq k$ or $k \leq \sqrt{v} \leq i - 1$). The duals of these designs are also E-optimal. In certain settings Partial Geometries are the unique E-optimal designs.

1. Introduction and notation. The object of this work is to investigate the E-optimality of certain discrete statistical experiments (chiefly PBIB designs) in the additive setting of the one way elimination of heterogeneity. For v, b, k positive integers, we denote by $\Omega_{v,b,k}$ the collection of all $k \times b$ arrays with varieties $1, 2, \cdots, v$ as entries ($2 \leq k < v$). Any such array $d \in \Omega_{v,b,k}$ is called a design. The columns of d are called blocks. A design is said to be binary if each block of d consists of distinct varieties; d is called equireplicated if each variety occurs the same numbers of times throughout the whole array d.

Let α_i be the unknown effect of variety i and β_j be the unknown effect of the jth block. In the additive model of elimination of heterogeneity in one direction, we assume that the expectation of an observation on variety i in the jth block of d is $\alpha_i + \beta_j$. The observations are assumed uncorrelated with common (unknown) variance σ^2. Our main interest is in comparing the variety effects $\alpha_1, \alpha_2, \cdots, \alpha_v$. The information matrix of variety effects under this model is

$$kC_d = k\,\mathrm{diag}(r_{d1}, \cdots, r_{dv}) - N_d N'_d$$

where $N_d = (n_{dij})$, with n_{dij} indicating the number of times variety i appears in the jth block of d; r_{di} is the replication number of variety i in d. J denotes the matrix with all its entries 1 and I is the identity matrix. By λ_{dij} we denote the (i, j)th entry of $N_d N'_d$. It is known that for any d, C_d is nonegative definite with row sums zero. Let further $0 = \mu_{d0} \leq \mu_{d1} \leq \cdots \leq \mu_{d,v-1}$ be the eigenvalues of C_d.

A design d^* is called E-optimal over $\Omega_{v,b,k}$ under this model, if the maximal variance of normalized best linear unbiased estimators of variety contrasts is minimal under d^*. In terms of eigenvalues, it is well-known that E-optimality deals with the association $d \to C_d \to \mu_{d1}$ and with the objective of finding a design d with maximal μ_{d1} over all of $\Omega_{v,b,k}$; see Ehrenfeld (1955) or Kiefer (1959, 1978).

In the next section we show that a design $d^* \in \Omega_{v,b,k}$ with $k\mu_{d^*1} \geq (v/(v - k))(r - 1)(k - 1)$ and $r = bkv^{-1}$ integral, is E-optimal. As a result, a number of families of PBIB designs (mentioned in the abstract) with λ_1 and λ_2 zero or one are proved E-optimal.

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2. Results. We denote by $\mathbf{1}$ the column vector with all its entries 1 and by J the (not necessarily square) matrix with all its entries 1. The following two lemmas provide upper bounds for μ_{d1}. Various bounds can also be found in Chakrabarti (1963), Jacroux (1980a, 1980b), Cheng (1980) or Constantine (1981).

LEMMA 2.1. *Let C be a $v \times v$ nonnegative definite matrix with zero row and column sums. Denote the eigenvalues of C by $0 = \mu_0 \le \mu_1 \le \cdots \le \mu_{v-1}$. Then the sum of entries in any $m \times m$ principal minor of C is at least $(m(v-m)/v)\,\mu_1$, $1 \le m \le v-1$.*

PROOF. Observe that a matrix obtained from C by row and (same) column permutations has the same eigenvalues as C. It will therefore be enough to prove the lemma for the $m \times m$ leading principal minor of C. Call this leading principal minor M. Then

$$\mathbf{1}'M\mathbf{1} = \left(\begin{pmatrix}\mathbf{1}\\0\end{pmatrix} - \frac{m}{v}\mathbf{1}\right)'C\left(\begin{pmatrix}\mathbf{1}\\0\end{pmatrix} - \frac{m}{v}\mathbf{1}\right) \ge \left(\begin{pmatrix}\mathbf{1}\\0\end{pmatrix} - \frac{m}{v}\mathbf{1}\right)'\left(\begin{pmatrix}\mathbf{1}\\0\end{pmatrix} - \frac{m}{v}\mathbf{1}\right)\mu_1 = \frac{m(v-m)}{v}\mu_1$$

as stated. The inequality relies on the known fact that

$$\mu_1 = \min_{x'1=0} \frac{x'Cx}{x'x}$$

and on observing that $\left(\begin{pmatrix}\mathbf{1}\\0\end{pmatrix} - \frac{m}{v}\mathbf{1}\right)'\mathbf{1} = 0$ (since the $\mathbf{1}$ in $\begin{pmatrix}\mathbf{1}\\0\end{pmatrix}$ is $m \times 1$). This ends the proof. □

Our next lemma gives an upper bound for μ_{d1} when $d \in \Omega_{v,b,k}$ is equireplicated.

LEMMA 2.2. *If an equireplicated design $d \in \Omega_{v,b,k}$ contains a block which consists of m distinct varieties, $2 \le m \le k$, then*

$$k\mu_{d1} \le \frac{v}{m(v-m)}(k-1)(mr-k).$$

PROOF. By eventually relabeling the varieties and reshuffling the blocks, we can assume that the first block in d consists of n_{d11} 1's, n_{d21} 2's $\cdots$ and n_{dm1} m's. Index the rows and columns of C_d by the varieties $1, 2, \cdots, v$ (in this order), and let M_d be the $m \times m$ leading principal minor of C_d. Observe, firstly, that $\sum_{j=1}^{b} n_{dij} = r$ and that

$$\sum_{j=1}^{b} n_{dij}^2 \ge n_{di1} + \sum_{j=2}^{b} n_{dij}^2 \ge \sum_{j=1}^{b} n_{dij} = r.$$

Hence $\sum_{j=2}^{b} n_{dij}^2 \ge r - n_{di1}$ and therefore $\sum_{j=1}^{b} n_{dij}^2 \ge n_{di1}^2 + r - n_{di1}$. Secondly, note that $\sum_{i\ne j}^{m} \lambda_{dij}$, which is a sum of $m(m-1)$ nonnegative terms, satisfies

$$\sum_{i=j}^{m} \lambda_{dij} = \sum_{i=j}^{m} \sum_{u=1}^{b} n_{diu}n_{dju} \ge \sum_{i\ne j}^{m} n_{di1}n_{dj1}.$$

Using these two inequalities and the fact that $\sum_{i=1}^{m} n_{di1} = k$, we obtain:

$$k\mathbf{1}'\mathrm{M}_d\mathbf{1} = mrk - \sum_{i=1}^{m}\sum_{j=1}^{b} n_{dij}^2 - \sum_{i\ne j}\lambda_{dij} \le mrk - \sum_{i=1}^{m}(n_{di1}^2 + r - n_{di1}) - \sum_{i\ne j}^{m} n_{di1}n_{dj1}$$

$$= mrk - \left(\sum_{i=1}^{m} n_{di1}\right)^2 - mr + \sum_{i=1}^{m} n_{di1} = (k-1)(mr-k).$$

That $k\mu_{d1} \le (v/m(v-m))(k-1)(mr-k)$ follows now from Lemma 2.1. This ends the proof. □

Through the remainder of the paper, let the varieties in a design $d \in \Omega_{v,b,k}$ be always labeled so that the replication numbers r_{di} satisfy $r_{d1} \le r_{d2} \le \cdots \le r_{dv}$. We now prove the following result:

THEOREM 2.1. *Let $r = bkv^{-1}$ be an integer. A design $d^* \in \Omega_{v,b,k}$ which satisfies $k\mu_{d^*1} \geq (v/(v-k))(r-1)(k-1)$ is E-optimal over $\Omega_{v,b,k}$ and its dual is E-optimal over $\Omega_{b,v,r}$.*

PROOF. Let d be any design in $\Omega_{v,b,k}$. Then d is either equireplicated or it is not. Suppose it is not. Then $r_{d1} \leq r - 1$ and by Lemma 2.1 with $m = 1$ we have

$$k\mu_{d1} \leq \frac{v}{v-1} r_{d1}(k-1) \leq \frac{v}{v-1}(r-1)(k-1) < \frac{v}{v-k}(r-1)(k-1) \leq k\mu_{d^*1},$$

which shows that such a design is strictly E-worse than d^*.

Assume now that d is equireplicated. We may also assume that d has a block which consists of m distinct varieties, $2 \leq m \leq k$. (Observe that if d has no such block, then the information matrix C_d is the zero matrix, and hence for such d we have $\mu_{d1} = 0 < \mu_{d^*1}$.) By Lemma 2.2 we can write

$$k\mu_{d1} \leq \frac{v}{m(v-m)}(k-1)(mr-k).$$

Let $Q(m) = -k\mu_{d^*1}m^2 + \{vk\mu_{d^*1} - v(k-1)r\}m + vk(k-1)$. Note that

$$\frac{v}{m(v-m)}(k-1)(mr-k) \leq k\mu_{d^*1},$$

for all $2 \leq m \leq k$ if and only if $Q(m) \geq 0$, for all $2 \leq m \leq k$. Since $Q(m)$ is a quadratic in m with negative leading coefficient and $Q(0) = vk(k-1) > 0$, checking that $Q(k) \geq 0$ would insure that $Q(m) \geq 0$ for all $2 \leq m \leq k$. By assumption $k\mu_{d^*1} \geq (v/(v-k))(r-1)(k-1)$ which implies $-k^2\mu_{d^*1} + vk\mu_{d^*1} - v(k-1)r + v(k-1) \geq 0$. In terms of Q this last inequality is simply $k^{-1}Q(k) \geq 0$. Since k is positive it follows that $Q(k) \geq 0$, as desired. We have therefore shown

$$k\mu_{d1} \leq \frac{v}{m(v-m)}(k-1)(mr-k) \leq k\mu_{d^*1},$$

for all $2 \leq m \leq k$. This shows the E-optimality of d^* over $\Omega_{v,b,k}$. That the dual of d^* is E-optimal over $\Omega_{b,v,r}$ follows from results of Shah, Raghavarao, Khatri (1976) and Cheng (1980, page 203).

All the Partially Balanced Incomplete Block designs which we shall prove E-optimal next, have E-optimal duals since (as we shall see) they satisfy the condition stated in Theorem 2.1.

Connor and Clatworthy (1954) found the nonzero eigenvalues of the information matrix of a PBIB design with two associate classes to be

$$k\mu_1 = r(k-1) + \tfrac{1}{2}\{(\lambda_1 - \lambda_2)(-\gamma + \sqrt{\Delta}) + \lambda_1 + \lambda_2\}$$

and

$$k\mu_2 = r(k-1) + \tfrac{1}{2}\{(\lambda_1 - \lambda_2)(-\gamma - \sqrt{\Delta}) + \lambda_1 + \lambda_2\}.$$

It is easy to see that $\mu_1 < \mu_2$ if and only if $\lambda_1 < \lambda_2$. γ and Δ are expressed in terms of the parameters of the association scheme as $\gamma = p_{12}^2 - p_{12}^1$ and $\Delta = (p_{12}^2 - p_{12}^1)^2 + 2(p_{12}^1 + p_{12}^2) + 1$; see Raghavarao (1971, page 126).

When specialized to PBIB designs Theorem 2.1 yields:

COROLLARY 2.1(a) *A Partially Balanced Incomplete Block design with $\lambda_1 = 0$, $\lambda_2 = 1$ and $\gamma - \sqrt{\Delta} + 1 \geq \dfrac{2(k-1)(rk-v)}{v-k}$ is E-optimal over all block designs*; (b) *A Partially Balanced Incomplete Block Design with $\lambda_1 = 1$, $\lambda_2 = 0$ and $1 - \gamma - \sqrt{\Delta} \geq \dfrac{2(k-1)(rk-v)}{v-k}$ is E-optimal over all block designs.*

It follows from this corollary that Partially Balanced Incomplete Block designs with parameters as below are E-optimal: (a) $\lambda_1 = 1$, $\lambda_2 = 0$, $t = k(k-1)(r-1)(v-k)^{-1}$ an integer, $p^1_{11} = (t-1)(r-1) + k - 2$ and $p^2_{11} = rt$; (b) Partial Geometries with two associate classes, as introduced by Bose (1963); (c) $\lambda_1 = 1$, $\lambda_2 = 0$ and $b < v$; (d) $\lambda_1 = 0$, $\lambda_2 = 1$, triangular scheme of size n and block size $k \geq (n/2) \geq 3$; (e) $\lambda_1 = 1$, $\lambda_2 = 0$, triangular scheme of size n and block size $k \geq n - 1$; (f) $\lambda_1 = 0$, $\lambda_2 = 1$, L_i association scheme and block size $k \geq \sqrt{v}$; (g) $\lambda_1 = 1$, $\lambda_2 = 0$, L_i association scheme and the block size k satisfying either $i - 1 \leq \sqrt{v} \leq k$ or $k \leq \sqrt{v} \leq i - 1$.

With regard to (c) the reader should also see Bose and Clatworthy (1955). They showed that any PBIB design with $\lambda_1 = 1$, $\lambda_2 = 0$ and $b < v$ necessarily has parameters as those listed in (a), above. Examples of such E-optimal PBIB designs can be found in the comprehensive tables of PBIB designs compiled by Clatworthy (1973) and the references given there.

With the exception of settings which allow BIB or Group Divisible designs with $\lambda_2 = \lambda_1 + 1$, an E-optimal design is in general not unique with this property. And though nonuniqueness prevails in general, if Partial Geometries exist in $\Omega_{v,b,k}$ they are the only E-optimal designs, provided that

$$bk(k-1)^2 > (k-3)v^2 + (k+1)v.$$

This follows by first observing that the first paragraph of Theorem 2.1 and Lemma 2.2 narrow down the search to the class of binary equireplicated designs in which any pair of varieties appears in at most one block. Now if a design d in this class is not a Partial Geometry (r, k, t), then it has a block B and a variety i not in B with the property that at least $t + 1$ blocks of d contain i and have nonempty intersection with B. Lemma 2.1 applied to the $(k+1) \times (k+1)$ principal minor of C_d determined by i and the other k varieties in B gives

$$k\mu_{d1} \leq v(k+1)^{-1}(v-k-1)^{-1}\{(k+1)r(k-1) - k(k-1) - 2t - 2\}.$$

When the numerical condition given above is satisfied, this last upper bound for $k\mu_{d1}$ is strictly less than $k\mu_{d^*1}$, where d^* is a Partial Geometry.

Let us illustrate our remarks on uniqueness by an example. $\Omega_{15,15,3}$ contains d^*, a partial Geometry of the symplectic type:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
d^*:	3	8	11	1	15	9	14	12	4	2	13	5	10	6	7
	6	3	5	7	10	15	11	13	2	14	9	4	1	12	8

Since the numerical condition is satisfied in this case, any E-optimal design in $\Omega_{15,15,3}$ must be a Partial Geometry.

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DEPARTMENT OF MATHEMATICS
INDIANA UNIVERSITY
BLOOMINGTON, INDIANA 47405