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E-OPTIMAL BLOCK DESIGNS UNDER HETEROSCEDASTIC MODEL

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ABSTRACT

This paper mainly studies the E-optimality of block designs under a general heteroscedastic setting. The C-matrix of a block design

under a heteroscedastic setting is obtained by using generalized least squares. Some bounds for the smallest positive eigenvalue of C-matrix are obtained in some general classes of connected designs. Use of these bounds is then made to obtain certain E-optimal block designs in various classes of connected block designs.

1. INTRODUCTION

This paper is mainly concerned with the determination and construction of some E-optimal block designs. In the usual setting of block designs, consider a design d with v treatments, n experimental units, and $N_d = (n_{dij})$ the $v x b_d$ incidence matrix, b_d being the number of blocks in d and n_{dij} the replication number of the ith treatment in the jth block of d, $i = 1,2,\ldots,v$; $j = 1,2,\ldots,b_d$. The ith row sum of N_d, r_{di}, is the replication of the ith treatment and the jth column sum of N_d, k_{dj}, is the size of the jth block. Also, $\sum_i r_{di} = n = \sum_j k_{dj}$. The fixed effects, additive statistical model assumed here for analysing the data obtained from a given design d specifies that the uth observation pertaining to the ith treatment in the jth block, y_{iju}, can be expressed as

$$y_{iju} = \mu + t_i + \beta_j + e_{iju}, \qquad u - 1,\ldots,n_{dij}, \qquad \ldots(1.1)$$

where μ is the general mean, t_i is the ith treatment effect and β_j is the jth block effect. Also e_{iju} is a random variable having expectation zero and variance-covariance structure as

$$\begin{aligned}
\mathrm{Cov}(e_{iju}, e_{i'j'u'}) &= \sigma^2\omega_j \,, && \text{if } j = j' \,,\ i = i' \,,\ u = u' \\
&= \sigma^2\rho \,, && \text{if } j = j' \text{ and either } i \neq i \text{ or } u \neq u' \\
&= 0 \,, && \text{if } j \neq j' \,. \qquad \ldots(1.2)
\end{aligned}$$

Here ω_j , ρ and σ^2 are constants such that $\omega_j > 0$, $|\rho| \leq 1$, $\sigma^2 > 0$, $\rho \neq \omega_j$ and $\rho \neq -\omega_j/(k_{dj}-1)$, $j = 1,\ldots,b_d$. It is reasonable to assume here that ω_j's are directly proportional to k_{dj}'s. Here we shall deal with only those models for which this assumption is valid. Under this model the coefficient matrix of the reduced normal equations for obtaining the generalized least square estimates of linear function of treatment effects is

$$C_d = \sum_{j=1}^{b_d} \frac{1}{\omega_j-\rho} [R_{dj} - \frac{1}{k_{dj}} N_{dj}N'_{dj}] \,, \qquad \ldots(1.3)$$

where N_{dj} is the jth column of N_d and $R_{dj} = \mathrm{diag}(n_{d1j},\ldots,n_{dvj})$. It is seen that C_d is symmetric, non-negative definite with zero row sums and for connected designs Rank $(C_d) = v-1$.

In this paper we shall only be concerned with designs which are connected. For given positive integers v , n , r_p , k_m , let $D(v,n,r_p,k_m)$ be the class of all connected block designs having v treatments, n experimental units, minimum replication of treatments, r_p , and maximum block size, k_m . Similarly, $D(v,n,r_p,k_1)$ will denote the class of all connected designs having v treatments, n units, minimum replication,

r_p , and minimum block size, k_1 , $D(v,n,k_m)$, the class of all connected designs with v treatments, n units and maximum block size, k_m and $D(v,n,k_1)$, the class of all connected block designs with v treatments, n units and minimum block size, k_1.

A design d^* in a given class $\mathfrak{D}$ of competing designs is said to be E-optimal in $\mathfrak{D}$ if and only if the smallest non-zero eigenvalue of C_{d^*} is at least as large as that of C_d for any other $d \in \mathfrak{D}$. It is well known that d^* is E-optimal if and only if it minimises the maximum variance of the least square estimators of normalized treatment contrasts.

A number of results are already known concerning the determination and construction of E-optimal block designs in various classes under the model where $\omega_j = 1$ and $\rho = 0$ (that is the usual homoscedastic and uncorrelated error model), e.g. see Takeuchi (1961), Cheng (1980), Constantine (1981,1982), Jacroux (1980a,b,1982,1983a,b), where the class of designs considered have blocks of equal size, while Lee and Jacroux (1987a,b,c), Pal and Pal (1988), Dey and Das (1989), Gupta and Singh (1989) also considered the class of designs having blocks of unequal size.

The assumption of constant variance σ^2 may not always hold if the block sizes are widely different and the intra block variance is dependent on block size. In such situations, one may assume an appropriate heteroscedastic model and use generalized least squares to obtain the best linear unbiased estimators of treatment contrasts. Recently some optimal block designs have been obtained under the heteroscedastic and uncorrelated error model (i.e. $\omega_j = k_j$ and $\rho = 0$) by Gupta, Das and Dey (1991).

Although a considerable amount of work is available for particular values of ρ and ω_j, viz., $\rho = 0$ and $\omega_j = 1$, in the error structure, not much appears to have been done in the optimality of block designs for general error structure. The purpose of this paper is to study the E-optimality of block designs with unequal block sizes when $\rho = 0$ and $\omega_j = k_{dj}^{1/\alpha}$ $(j=1,\ldots,b_d)$, $\alpha \in (0,\infty]$ is a constant. In Section 2, upper and lower bounds to the smallest non-zero eigenvalue of C_d with d belonging to different classes of connected designs is obtained. Use of these bounds is made in Section 3 to derive several classes of E-optimal designs. Finally in Section 4 optimality of designs with equal or unequal block sizes when $\rho \in (0,1)$ and $\omega_j = 1$ are reported.

2. BOUNDS FOR μ_{d1}

In this section, we obtain some bounds for μ_{d1}, the smallest positive eigenvalue of C_d, with d belonging to different classes of connected designs.

We consider $\rho = 0$. Also we assume that the variability of the observations obtained from a given block of the design d is an increasing function of the size of the block, i.e., $\omega_j = f(k_j)$, where $f(.)$ is an increasing function. In particular we consider the case where $\omega_j = k_{dj}^{1/\alpha}$, $\alpha \in (0,\infty]$ is a constant.

Theorem 2.1 Let $\rho = 0$, $\omega_j = k_{dj}^{1/\alpha}$, $d \in D(v,n,r_p,k_m)$ with $k_m \leq \alpha + 1$. Then

$$\mu_{d1} \leq \frac{r_p(k_m - 1)v}{(v-1)k_m^{1+1/\alpha}} . \qquad \ldots(2.1)$$

Proof Let x_i be a v-component column vector with ith entry equal to $(1 - 1/v)$ and all other entries equal to $-1/v$. Then it is easy to observe that $1_v' x_i = 0$ and $x_i' C_d x_i = c_{dii}$ where 1_s is an s-component column vector of unities and c_{dii} is the ith diagonal element of C_d. Thus,

$$\mu_{d1} \leq x_i' C_d x_i / x_i' x_i = v c_{dii}/(v-1) . \qquad \ldots(2.2)$$

Now from (1.3)

$$c_{dii} = \sum_{j=1}^{b_d} \frac{n_{dij}}{k_{dj}^{1/\alpha}} - \sum_{j=1}^{b_d} \frac{n_{dij}^2}{k_{dj}^{1+1/\alpha}}$$

$$\leq \sum_{j=1}^{b_d} n_{dij} \frac{1}{k_{dj}^{1/\alpha}} \left(1 - \frac{1}{k_{dj}}\right) . \qquad \ldots(2.3)$$

The function $\frac{1}{k_{dj}^{1/\alpha}} \left(1 - \frac{1}{k_{dj}}\right)$, $j = 1,\ldots,b_d$, $d \in D(v,n,k_m)$ has a maximum value $(k_m - 1)/k_m^{1+1/\alpha}$ if $k_m \leq \alpha + 1$. Therefore from (2.3), we have

$$c_{dii} \leq \frac{k_m - 1}{k_m^{1+1/\alpha}} \sum_{j=1}^{b_d} n_{dij} = \frac{r_{di}(k_m - 1)}{k_m^{1+1/\alpha}} . \qquad \ldots(2.4)$$

Since (2.4) holds for all $i = 1,\ldots,v$, (2.1) follows.

Theorem 2.2 Let $d \in D(v,n,k_m)$. Then

$$\mu_{d1} \geq \frac{\lambda_{dp} v}{k_m(\omega_m - \rho)}, \qquad \ldots(2.5)$$

where λ_{dp} is the smallest off-diagonal element of $N_d N_d' = (\lambda_{dij})$, $\rho \in (0,1)$ and $\omega_m = f(k_m)$, $f(.)$ an increasing function.

Proof Following Jacroux (1980b), let

$$T_{xd} = k_m(\omega_m - \rho)\, C_d - xv(v-1)^{-1} (I_v - v^{-1} 1_v 1_v') \qquad \ldots(2.6)$$

where I_v is the vth order identity matrix and x is a real number. The eigenvalues of T_{xd} are zero and $k_m(\omega_m - \rho)\, \mu_{di} - xv(v-1)^{-1}$, $i = 1,\ldots,v-1$, where $\mu_{d1} \leq \mu_{d2} \leq \cdots \leq \mu_{d,v-1}$ are the positive eigenvalues of C_d. If $T_{xd} = (t_{xduw})$, then

$$t_{xduu} = k_m(\omega_m - \rho) \sum_{j=1}^{b_d} \frac{1}{\omega_j - \rho} \left(n_{duj} - \frac{1}{k_{dj}} n_{duj}^2\right) - x$$

$$t_{xduw} = -k_m(\omega_m - \rho) \sum_{j=1}^{b_d} \frac{n_{duj}\, n_{dwj}}{k_{dj}(\omega_j - \rho)} + x(v-1)^{-1} \qquad \ldots(2.7)$$

Now, since $C_d 1_v = 0$, we have $T_{xd} 1_v = 0$, i.e.,

$$k_m(\omega_m - \rho) \sum_{j=1}^{b_d} \frac{1}{\omega_j - \rho} (n_{duj} - \frac{1}{k_{dj}} n_{duj}^2)$$

$$- k_m(\omega_m - \rho) \sum_{u(\neq w)}^{v} \sum_{j=1}^{b_d} \frac{n_{duj} n_{dwj}}{k_{dj}(\omega_j - \rho)} = 0, \quad u = 1,\ldots,v;$$

$$\Rightarrow \quad k_m(\omega_m - \rho) \sum_{j=1}^{b_d} \frac{1}{\omega_j - \rho} (n_{duj} - \frac{1}{k_{dj}} n_{duj}^2) - \lambda_{dp}(v-1) \geq 0 \quad \ldots(2.8)$$

Thus, for $x = \lambda_{dp}(v-1)$, we get from (2.7) and (2.8)

$$t_{xduu} \geq 0 \quad \text{for} \quad u = 1,\ldots,v$$

and

$$t_{xduw} \leq 0 \quad \text{for} \quad u \neq w,\ u,\ w = 1,\ldots,v\ . \quad \ldots(2.9)$$

The rest of the proof follows from Jacroux (1980b, p.663).

From Theorems 2.1 and 2.2, we have the following results.

Corollary 2.1 Let $\rho = 0$, $\omega_j = k_{dj}^{1/\alpha}$, $d \in D(v,n,r_p,k_m)$ with $k_m \leq \alpha+1$. Then,

i) $\lambda_{dp} v / k_m^{1+1/\alpha} \leq \mu_{d1} \leq \dfrac{r_p(k_m - 1)v}{(v-1)k_m^{1+1/\alpha}}$

ii) If $\lambda_{dp} = r_p(k_m - 1)/(v-1)$, then

$\mu_{d1} = \dfrac{r_p(k_m - 1)v}{(v-1)k_m^{1+1/\alpha}}$ and d is E-optimal in $D(v,n,r_p,k_m)$.

Corollary 2.2 Let $\rho = 0$, $\omega_j = k_{dj}^{1/\alpha}$, $d \in D(v,n,k_m)$ with $k_m \leq \alpha+1$. Then,

i) $\lambda_{dp} v / k_m^{1+1/\alpha} \leq \mu_{d1} \leq \dfrac{\bar{r}(k_m - 1)v}{(v-1)k_m^{1+1/\alpha}}$

where λ_{dp} is the smallest off-diagonal element of $N_d N_d'$ and $\bar{r}$ is the largest integer not exceeding n/v.

ii) If $\lambda_{dp} = \bar{r}(k_m - 1)/(v-1)$, then

$$\mu_{d1} = \frac{\bar{r}(k_m - 1)v}{(v-1)k_m^{1+1/\alpha}} \quad \text{and } d \text{ is E-optimal in } D(v,n,k_m).$$

Remark 1 The above results are generalizations of those known in the homoscedastic case. When $\alpha \longrightarrow \infty$, the results hold for the homoscedastic and uncorrelated error model as considered by Lee and Jacroux (1987a,b,c), Pal and Pal (1988), Dey and Das (1989) and Gupta and Singh (1989). For $\alpha \longrightarrow \infty$, the classes considered here are more general than the ones considered by Lee and Jacroux (1987a,b,c) and Pal and Pal (1988).

Above we have developed bounds for μ_{d1} with specified *maximum* block size k_m. Now we obtain bounds for μ_{d1} where d belongs to the class of designs with specified *minimum* block size k_1.

Theorem 2.3 Let $\rho = 0$, $\omega_j \doteq k_{dj}^{1/\alpha}$, $d \in D(v,n,r_p,k_1)$ with $k_1 \geq \alpha + 1$. Then

$$\mu_{d1} \leq \frac{r_p(k_1 - 1)v}{(v-1)k_1^{1+1/\alpha}} . \quad \ldots(2.10)$$

Proof On lines similar to Theorem 2.1, we have

$$\mu_d \leq \frac{v}{v-1} \sum_{j=1}^{b_d} n_{dij} \frac{1}{k_{dj}^{1/\alpha}} \left(1 - \frac{1}{k_{dj}}\right). \qquad \ldots(2.11)$$

The function $\frac{1}{k_{dj}^{1/\alpha}} \left(1 - \frac{1}{k_{dj}}\right)$, $j = 1,\ldots,b_d$, $d \in D(v,n,k_1)$ has a maximum value $(k_1 - 1)/k_1^{1+1/\alpha}$ if $k_1 \geq \alpha + 1$. Therefore from (2.11), we have

$$\mu_{d1} \leq \frac{v(k_1-1)}{(v-1)k_1^{1+1/\alpha}} \sum_{j=1}^{b_d} n_{dij} = \frac{r_{di}(k_1-1)v}{(v-1)k_1^{1+1/\alpha}}. \qquad \ldots(2.12)$$

Since (2.12) holds for all $i = 1,\ldots,v$, (2.10) follows.

Corollary 2.3 Let $\rho = 0$, $\omega_j = k_{dj}^{1/\alpha}$, $d \in D(v,n,k_1)$ with $k_1 \geq \alpha + 1$. Then

$$\mu_{d1} \leq \frac{\bar{r}(k_1-1)v}{(v-1)k_1^{1+1/\alpha}}. \qquad \ldots(2.13)$$

where $\bar{r}$ is the largest integer not exceeding n/v.

Theorem 2.3 and Corollary 2.3 give upper bounds for μ_{d1} when $\alpha \leq k_1-1$. Thus, these bounds do not hold for the homoscedastic case. However, these bounds holds for situations where the variance is truely dependent on block size and α is small, say, less than 3.

Remark 2 It is to be noted that a design which is E-optimal in $D(v,n,k_m)$ $(D(v,n,k_1))$ is also E-optimal in $D(v,b,k_1,\ldots,k_b)$, the class of all connected block designs having v treatments, b blocks and specified block sizes $k_1,\ldots,k_b$, provided the design belongs to $D(v,b,k_1,\ldots,k_b)$ with $\max(k_1,\ldots,k_b) = k_m$ $(\min(k_1,\ldots,k_b) = k_1)$. The class of competing designs considered here is very broad since it only specifies (apart from v and n) either the maximum or the minimum block size.

3. E-OPTIMAL DESIGNS

In this section we give some methods of constructing E-optimal block design under the heteroscedastic uncorrelated error model, i.e., the case $\rho = 0$ and $\omega_j = k_{dj}^{1/\alpha}$, $j = 1,\ldots,b_d$.

Let d_1 be a Balanced Incomplete Block (BIB) design with parameters v, b, r, k, λ, in short $BIB(v,b,r,k,\lambda)$, and the treatments be $0,1,2,\ldots,v-1$. This design has bk experimental units. Suppose $n'(\geq 1)$ more experimental units are available to the experimenter. The problem then is to derive an E-optimal design for v treatments and $n=bk+n'$ experimental units. The cases (i) $\alpha \geq k-1$ and (ii) $\alpha \leq k-1$ are dealt separately.

Case (i) : $\alpha \geq k-1$

As a consequence of Corollaries 2.1 and 2.2, we have

Theorem 3.1 Let d_1 be a BIB(v,b,r,k,λ), $k \leq \alpha+1$ and let d_2 be any arbitrary design with $v' < v$ treatments, n' experimental units and maximum block size $\leq k$. Then the design d^* with $n = bk+n'$ experimental units and maximum block size $k_m = k$, obtained by taking the union of d_1 and d_2 is

i) E-optimal in $D(v,n,r_p,k_m)$ with $r_p = r$, $k_m = k$.

ii) E-optimal in $D(v,n,k_m)$ if $n' < v$.

The above result is very general. To give some discrete structure to the design d^* , we suggest specific d_2.

The design d_2 is having n' experimental units grouped into b' blocks, the blocks being of size atmost k, where,

$$b' = [n'/k] + 1, \qquad \text{if } k \nmid n'$$
$$= n'/k , \qquad \text{if } k \mid n' .$$

To the b blocks of d_1 , let us add b' blocks in the following manner so as to get a design d^* in $b+b'$ blocks.

i) If $n' < k$, we just add one block of size n' having treatments with labels $0,1,\ldots,n'-1$.

ii) If $n' = mk$ for some integer $m(\geq 1)$, we add $b' = m$ blocks, each of size k. The contents of first of these blocks are $(0,1,2,\ldots,k-1)$ and rest of the blocks are obtained by 'developing' this block in steps of k, with elements reduced mov$(v-1)$.

iii) If $n' > k$ but $k \nmid n'$, let $n' = mk+c$, $1 \leq c \leq k-1$. In this this case, we construct m blocks, each of size k, as in (ii) above. The last block has size c and contains treatments $(i+1,i+2,\ldots,i+c)$, where i is the label of the last treatment in the m-th block, the elements being reduced $\bmod(v-1)$.

Another alternative is to take d_2 as a BIB or PBIB design with $v'(< v)$ treatments, b' blocks each of size $k'(< k)$ where $n' = b'k'$.

The design d^* obtained from the above specific d_2 is E-optimal in $D(v,bk+n',r,k)$ and if $n' < v$ is E-optimal in $D(v,bk+n',k)$.

Case (ii) : $\alpha \leq k-1$

Theorem 3.2 Let d_1 be a $BIB(v,b,r,k,\lambda)$, $k \geq \alpha+1$, and d_3 is an arbitrary design with $v' < v$ treatments, n' experimental units and minimum block size $\geq k$, then the design d^{**} with $n = bk+n'$ experimental units and minimum block size $k_1 = k$ obtained by taking the union of d_1 and d_3 is

i) E-optimal in $D(v,n,r_p,k_1)$ with $r_p = r$, $k_1 = k$.

ii) E-optimal in $D(v,n,k_1)$ if $n' < v$.

Proof It is easy to see that $\mu_{d^{**}1} = \dfrac{r(k-1)v}{(v-1)k^{1+1/\alpha}}$. The result then follows from Theorem 2.3 and Corollary 2.3.

As in Case (i), here also we may consider specific d_3 . For example, d_3 can be taken as a BIB or PBIB design with $v'(< v)$ treatments, b' block, each of size $k'(> k)$.

Remark 3 Starting with a BIB design with block size k, if we have n' more experimental units, then depending on whether $\alpha \geq k-1$ or $\alpha \leq k-1$, we use Theorem 1 or 2 respectively. For $\alpha \geq k-1$, the arbitrary design d_2 with $k_m \leq k$ is used and for $\alpha \leq k-1$, the arbitrary design d_3 with $k_1 \geq k$ is used.

Remark 4 Gupta, Das and Dey (1991) have shown the universal optimality of variance balanced design for $\alpha = 1$ or ∞ . This can be generalized to any value of $\alpha \in (0,\infty]$. The universal optimality of variance balanced designs for $\omega_j = k_j^{1/\alpha}$, $\alpha \in (0,\infty]$ will be reported in a separate communication.

4. OPTIMAL DESIGNS UNDER CORRELATED ERROR MODEL

In this section we shall consider the case for which $\rho \in (0,1)$ and $\omega_j = 1$, $j = 1,\ldots,b_d$, i.e., the homoscedastic and correlated error model. It is shown that under the above set up, the search for optimal designs under correlated error model reduces to that under uncorrelated error model.

From the expression given in (1.3) when $\omega_j = 1$, $j = 1,\ldots,b_d$ and $\rho \in (0,1)$, we have

$$C_d = \frac{1}{1-\rho} \sum_{j=1}^{b_d} [R_{dj} - \frac{1}{k_{dj}} N_{dj}N'_{dj}]$$

$$= \frac{1}{1-\rho} C_{d(o)} \qquad \ldots(4.1)$$

where $C_{d(o)}$ is the C-matrix of the design d under homoscedastic and uncorrelated error model. Let D be the class of connected designs under study. Then from (4.1) we have

Theorem 4.1 For $\rho = 0$ and $\omega_j = 1$, if $d^* \in D$ is ϕ-optimal according to a non-increasing optimality criterion ϕ, then d^* is also ϕ-optimal under the model with $\rho \in (0,1)$ and $\omega_j = 1, j = 1,\ldots,b_d$. [An optimality criterion ϕ is non-increasing if $\phi(A) \leq \phi(B)$, whenever $A-B$ is non-negative definite].

Remark 5 The ϕ-optimality criterion includes the A-, D- and E-optimality criterion. The various optimal designs in literature (including the ones in Section 3) obtained under the uncorrelated and homoscedastic error model are also optimal for $\rho \in (0,1)$.

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