

On The A-, D- And E-Optimality of PBNB Designs

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This paper extending to n-ary block of Soundarapandian (1980a), a partially balanced n-ary Block (PBNB) design discussed.

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I. Introduction

E-optimality of some statistical experiments (both BNB and PBNB designs) in additive one-way elimination of heterogeneity. Here $D(V.B.K.)$ represents the collection of all $K \times B$ arrays with treatments $1, 2, \dots, V$. Any such array $d \in D(V.B.K.)$ is a n-ary design. A design is said to be n-ary if each block of d consists of treatments; d is called equireplicated, if each variety occurs the same number of times throughout the whole array d .

The additive model of elimination of heterogeneity in one direction, we assume that the expectation of an observation on variety i in the j -th block of d is $\alpha_i + \beta_j$. The observations are assumed uncorrelated with common variance (unknown) σ^2 .

The information matrix of treatment effect is

$$KC_d = K \text{diag} (R_{d1} R_{d2} \dots R_{dV}) - N_d N_d'$$

Where $N_d = (n_{dij})$. With n_{dij} indicating the number of times treatment i appears in the block of d . Our main interest is to compare the treatments $(\alpha_1, \alpha_2, \dots, \alpha_v)$ of n-ary design d . Here R_{di} is replication of treatment i in d . j denotes the matrix with as entries I and I is the identity matrix. Λ_{dij} denote the (i,j) -th entry of $N_d N_d'$ as known that for any d , C_d is nonnegative definite with row sums zero. Let further

$$0 = \mu_{d0} \leq \mu_{d1} \leq \dots \leq \mu_{dv-1}$$
 in the eigen values of C_d

II. Preliminary Results

Some inequalities and parameter relations of PBNB designs and further results have been worked out after considering the concepts of BNB, PBNB designs and E- optimality criterion.

Following Tocher (1952) and later for inequality $B \geq V$ by Soundarapandian (1980a), define a balanced n-ary block (BNB) design as an arrangement of V -treatments in B blocks each of size K , such as the i^{th} treatment occurs in the j^{th} block n_{ij} times, and altogether R times, when n_{ij} can take values $0, 1, 2, \dots, (n-1)$. We say that the design is variance balanced if the inner product of any two new vectors of the incidence matrix,

$N_{V \times B}$ of the n-ary design $\sum_{i=1}^B n_{ij} n_{kj}$ is a constant and equal to Λ (say) for all $i = k = 1, 2, 3, \dots, v$. This implies

$$\text{also that } \sum_{i=1}^B n_{ij}^2 = \Delta, \text{ (another constant) for all } i=1, 2, 3, \dots, v.$$

According to Hedayat and Federer (1974), a n-ary block design is said to be pairwise balance if $NN' = D(\Delta) + \Lambda J$, when N' is the transpose of the incidence matrix N , D a diagonal form of matrix with elements Δ , Λ a scalar and J matrix with unit entries everywhere.

Generalizing the definition of ternary block design of Paik and Federer (1973) and Mehta, Agarwal and Nigam (1975) and extending to n-ary block of Soundarapandian (1980a), a partially balanced n-ary Block (PBNB) design is defined in the following lines.

Definition:

A block design with V treatments B blocks is said to be a Partially balanced n-ary block (PBNB) design with m associate classes if

- (i) the incidence matrix $N_{V \times B}$ has n entries $0, 1, 2, \dots, (n-1)$,
- (ii) $\sum n_{ij} = K$ for every $j=1, 2, \dots, B$.
- (iii) $\sum n_{ij} = R$ and $\sum n_{ij}^2 = \Delta$ and, for every $i=1, 2, \dots, V$.

- (iv) there exists a relationship between the treatments defined as:
 - (a) any two treatments are either 1st 2nd,.....or mth associates, the relation of association being symmetrical
 - (b) each treatment. 'a' has n_xα-th associates, then the number of treatments that are j-th associates of 'a' and k-th associates of 'd' is P^α_{ij} and is independent of the pair of α-th associates 'a' and 'd'.
- (v) the inner product of any two rows of N, ie $\sum_{j=1}^B n_{ij} n_{kj} = \Lambda_\alpha$ if i and i' are mutually α- th associate, α = 1,2,.....m.

Paik and Federer (1973) and Soundarapandian (1980a) introduced partially balanced n-ary block designs (PBNBD) as natural extension of BNBD's which had intuitively attracted combinatorial properties and whose algebraic properties enabled efficiency factor to be easily calculated. More attention has been paid to PBNBD's with two associate classes, hereafter called PBNB (2) designs. An alternative approximation to combinatorial balanced is to have precisely two non-trivial concurrences, which differ by one or a scalar quantity. Any such designs are called PBNB designs and not a BNB design.

In the above model, a design d* is called E-Optimal over D (V,B,K). if the maximal variance of normalized best linear unbiased estimators of treatment contrast is minimal under d*. In terms of eigenvalues, it is well known that E-optimality deals with the association $d \rightarrow C_d \rightarrow \mu_{d1}$ and with the objective of finding a design d with maximal μ_{d1} over all of D (V.B.K) – as per the extension of binary to n-ary from Eherenfeld (1955) or Kiefer (1959,1978).

III. Various Bounds For BNBA and PBNB Designs

Following the contributions of Soundrapandian(1980 a,b) one can arrive various bounds for n-ary block design by using the bounds for binary design which have been discussed by Constantine (1982).

Lemma:

Let C be a (VxV) non-negative definite matrix with zero row and column sums. The eigenvalues of C be $0 = \mu_0 \leq \mu_1 \leq \mu_2 \dots \leq \mu_{v-1}$. Then the sum of entries in any (m x m) principal minor of C is at least. $\{m(V-m)/V\} \mu_1$; $1 \leq m \leq (v-1)$

Proof:

The leading principal minor M of C which has row and column permutation has the same eigenvalues in C. Then.

$$\begin{aligned}
 \text{Tr}MI &= \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{m}{V} \mathbf{1} \right)' C \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{m}{V} \mathbf{1} \right) \\
 &\geq \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{m}{V} \mathbf{1} \right)' \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{m}{V} \mathbf{1} \right) \mu_1 = \frac{m(V-m)}{V} \cdot \mu_1
 \end{aligned}$$

where $\mathbf{1}$ represents the column vector with all its entries 1. The inequality relies on the known fact that

$$\mu_1 = \text{Min}_{x'1=0} \frac{x'Cx}{x'x}$$

Also

$$\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{m}{V} \mathbf{1} \right)' \mathbf{1} = 0 \text{ (since the } \mathbf{1} \text{ in } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ is } m \times 1).$$

Thus we get the result proved.

For an equireplicated n-ary design $d \in D (V,B,K)$, we get the upper bound for μ_{d1} as in the following lemma.

Lemma:

If an equi-replicated n-ary block design $d \in D(V, B, K)$ contains a block which consists of m treatments, $2 \leq m \leq K$, then

$$K\mu_{d1} \leq \frac{V}{m(V-m)} (K-1)(mR-K)$$

Proof:

Let the first block in d consists of n_{d11} 1's, n_{d21} 2's..... and n_{dm1} m 's. Index the rows and columns of C_d by the treatments 1,2,3,..... V (in this order)

Let M_d be the $(m \times m)$ leading principal minor of C_d . Here $\sum_{j=1}^B n_{dij} = R$ and that

$$\Delta = \sum_{j=1}^B n_{dij}^2 \geq n_{d11}^2 + \sum_{j=2}^B n_{dij}^2 \geq \sum_{j=1}^B n_{dij}^2 = R$$

Hence

$$\Delta = \sum_{j=2}^B n_{dij}^2 \geq R - n_{d11}^2$$

and so

$$\Delta = \sum_{j=1}^B n_{dij}^2 \geq n_{d11}^2 + R - n_{d11}^2$$

Secondly $\sum_{i=1}^m \Lambda_{dij}$ which is a sum of $m(m-1)$ non-negative terms.

Thus

$$\sum_{i=j}^m \Lambda_{dij} = \sum_{i=j}^m \sum_{u=1}^B n_{diu} n_{dju} \geq \sum_{i=j}^m n_{dij} n_{dji}$$

From the two inequalities, and using the fact that $\sum_{i=1}^m \Lambda_{dij} = K$, we get,

$$\begin{aligned} K1'M &= mRK - \sum_{i=1}^m \sum_{j=1}^B n_{dij}^2 - \sum_{i \neq j} \Lambda_{dij} \\ &\geq mRK - \sum_{i=1}^m (n_{d1i}^2 + \Delta - n_{d1i}^2) \sum_{i \neq j} n_{d1i} n_{d1i} \\ &= mRK - \left(\sum_{i=1}^m n_{dij} \right)^2 - mR + \sum_{j=1}^B n_{dij} \\ &= (K-1)(mR-k) \end{aligned}$$

Thus $K\mu_{d1} \leq \{V/m(V-m)\} \{K-1\}(mR-k)$ follows from lemma (5.3.1). Thus we proves the lemma.

In future, let $R_{d1} \leq R_{d2} \leq R_{d3} \leq \dots R_{dV}$

Then we have the following theorem:

Theorem:

Let $R = \frac{BK}{V}$ be an integer. A design $d^* \in D(V, B, K)$, which satisfies

$K\mu_{d^*} \geq \frac{V}{V-K} (R-1) (K-1)$ is E-Optimal over $D(V, B, K)$ and its dual is E-Optimal over $D(V, B, K)$.

Proof:

Let d be any design in $D(V, B, K)$

Let also that d is either equireplicated or it is not. Suppose it is not equireplicated, then $R_{d_i} \leq (R-1)$. By Lemma (5.3.1) with $m=1$, we have,

$$K\mu_{d_i} \leq \frac{V}{V-1} R_{d_i} (K-1) \leq \frac{V}{V-1} (R-1) (K-1) < \frac{V}{V-K} (R-1) (K-1) \leq K\mu_{d^*}$$

Thus, this kind of design is strictly E less Optimal than d^*

IV. Assume That D Is Equireplicated:

Let d has a block which consists of m distinct treatments, $2 \leq m \leq K$. Then C_d is the zero matrix.

For such d , we have $\mu_{d_i} = 0 < \mu_{d^*}$.

By Lemma (5.3.2), we have

$$K\mu_{d_i} \leq \frac{V}{m(V-m)} (K-1) (mR-K)$$

$$\text{Let } S(m) = -K\mu_{d^*} m^2 + \{VK\mu_{d^*} - V(K-1)R\} m + VK(K-1)$$

Note that $\frac{V}{m(V-m)} (K-1) (mR-K) \leq K\mu_{d^*}$ for all $2 \leq m \leq K$, if and only if $S(m) \geq 0$ for all $2 \leq m \leq K$.

Since $S(m)$ is a quadratic in m with negative leading coefficients and $S(0) = VK(K-1) > 0$. Finding that $S(K) \geq 0$, would give that $S(m) > 0$ for all $2 \leq m \leq K$. Form the assumption.

$$K\mu_{d^*} \geq \left\{ \frac{V}{(V-K)(R-1)} \right\} (R-1) (K-1), \text{ we get}$$

$$-K^2\mu_{d^*} + VK\mu_{d^*} - V(K-1)R + V(K-1) \geq 0$$

In terms of S , the inequality simplifies to

$$K^{-1} S(K) \geq 0$$

Since K is positive, it follows that $S(K) \geq 0$. Then we can show that

$$K\mu_{d_i} \leq \frac{V}{m(V-m)} (K-1) (mR-K) \leq K\mu_{d^*}, \text{ for all } 2 \leq m \leq K.$$

This result shows the E-Optimality of d^* on $D(V, B, K)$

Corollary

The dual of d^* of Theorem (5.3.3), is E-Optimal over $D(V, B, K)$

Proof:

Following the binary results of Shah, Raghavarao, Khatri (1976) and Cheng (1980a) and extending to n-ary block designs of Soundapandian (1980a), we can prove that the dual of d^* in Theorem (5.3.3) is E-Optimal over D (V,B,K).

V. E-Optimal PBNB Designs

Cannor and Clatworthy (1954) found the non-zero eigenvalues of the information matrix of a PBIB design with two associate classes to be

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

and

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

Where $\gamma = P^2_{12} - P^1_{12}$ and $\Delta = (P^2_{12} - P^1_{12})^2 + 2(P^2_{12} - P^1_{12})$

Now utilizing the result of PBNB designs of Soundarapandian's thesis (1981d), we get the two non-zero eigenvalues of the information matrix of PBNB designs with two associate classes are:

$$K\mu_1 = (RK - \Lambda_0) - \frac{1}{2} \{ (\Lambda_1 \cdot \Lambda_2) (-\gamma + \sqrt{\Delta}) + \Lambda_1 + \Lambda_2 \}$$

and

$$K\mu_2 = (RK - \Lambda_0) + \frac{1}{2} \{ (\Lambda_1 \cdot \Lambda_2) (-\gamma - \sqrt{\Delta}) + \Lambda_1 + \Lambda_2 \}$$

Where $\gamma = P^2_{12} - P^1_{12}$, $\beta = P^2_{12} - P^1_{12}$, $\Delta = \gamma^2 + 2\beta + 1$
(Difference between Λ and Λ_0 can be noticed.)

If $\Lambda_1 < \Lambda_2$ we can easily see that $\mu_1 < \mu_2$, and now we get the following theorem.

Theorem:

- (a) A partially Balanced n-ary block (PBNB) designs with $\Lambda_1 = 0$, $\Lambda_2 = a$ (a is a scalar quantity may take any values) and

$$\gamma - \sqrt{\Delta} + a \geq \frac{2(K-1)(RK-V)}{(V-K)} \text{ is E-Optimal over all n-ary block designs}$$

- (b) A partially Balanced n-ary block (PBNB) design with $\Lambda_1 = a$, $\Lambda_2 = 0$ (where a is a scalar quantity may take value) and

$$a + \gamma - \sqrt{\Delta} \geq \frac{2(K-1)(RK-V)}{(V-K)} \text{ is E-Optimal over all block designs.}$$

Proof:

Utilizing the theorem (5.3.3), the proof of the theorem follows for PBNB designs.

From the above Theorem (5.4.1), we can see the following PBNB designs with 2 associate classes with the following parameters are E-Optimal.

- (a) $\Lambda_1 = a$, $\Lambda_2 = 0$, $t = K(K-1)(R-1)(V-K)$ an integer and $P^1_{11} = (t-1)(R-1) + (K-2)$ and $P^2_{11} = R_t$.
- (b) Bose's (1963) partial geometries with two associate classes are E-Optimal PBIB designs, which can be extended to E-Optimal PBIB designs.
- (c) $\Lambda_1 = a$, $\Lambda_2 = 0$ and $B < V$.
- (d) $\Lambda_1 = a$, $\Lambda_2 = 0$ triangular scheme of size n and block size $K \geq n-1$.
- (e) $\Lambda_1 = 0$, $\Lambda_2 = a$, L_1 association scheme and block size $K \geq \sqrt{V}$
- (f) $\Lambda_1 = a$, $\Lambda_2 = 0$, L_1 association scheme and block of size K satisfying either $(i-1) \leq \sqrt{V} \leq K$ (or) $K \leq \sqrt{V} \leq (i-1)$

For (c), it is very difficult to find PBNP design but for PBIB designs, we can find from Bose and Clatworthy (1955). Examples of E-Optimal PBIB design are found from tables of PBIB designs compiled by Clatworthy (1973) and this can be used.

Example:

Blocks	Treatments	Blocks	Treatments	Blocks	Treatments
1	1 1 3 6	16	6 6 9 15	31	11 11 13 9
2	1 3 3 6	17	6 9 9 15	32	11 13 13 9
3	1 3 6 6	18	6 9 15 15	33	11 13 9 9
4	2 2 8 3	19	7 7 14 11	34	12 12 5 4
5	2 8 8 3	20	7 14 14 11	35	12 5 5 4
6	2 8 3 3	21	7 14 11 11	36	12 5 4 4
7	3 3 11 5	22	8 8 12 13	37	13 13 10 1
8	3 11 11 5	23	8 12 12 13	38	13 10 10 1
9	3 11 5 5	24	8 12 13 13	39	13 10 1 1
10	4 4 1 7	25	9 9 4 2	40	14 14 6 12
11	4 1 1 7	26	9 4 4 2	41	14 6 12 12
12	4 1 7 7	27	9 4 2 2	42	14 6 12 12
13	5 5 15 10	28	10 10 2 14	43	15 15 7 8
14	5 15 15 10	29	10 2 2 14	44	15 7 7 8
15	5 15 10 10	30	10 2 14 14	45	15 7 8 8

VI. Further PBNB Designs

Let $D(V,B,K)$ be the set of n -ary equireplicate incomplete block designs for V treatments in B blocks of size K . For any $d \in D(V,B,K)$, let N_d be the $V \times B$ treatment block incidence matrix of d . Then the information matrix of d in a new form can be given as:

$$C_d = RI - K^{-1} N_d N_d'$$

The matrix $N_d N_d'$ is called the concurrence matrix of d and its off-diagonal entries as nontrivial concurrences. C_d is symmetric, non-negative definite and has zero row sums.

Let $0 = \mu_{d0} \leq \mu_{d1} \leq \dots \leq \mu_{dV}$ be the eigenvalues of C_d . Then Commonly used A, D and E-Optimality criterion seek to minimize.

$$\sum_{i=1}^{V-1} (\mu_{di})^{-1}, \prod_{i=1}^{V-1} (\mu_{di})^{-1} \text{ and } (\mu_{dV-1})^{-1} \text{ respectively.}$$

As per Kiefer (1975) if $D(V,B,K)$ has d^* is having non-trivial concurrences equal, then d^* is universally optimal n -ary block designs over $D(V,B,K)$, in particular, they are A, D and E-Optimal over $D(V,B,K)$.

We have already defined a Partially Balanced n -ary. Block (PBNB) design. Now we proceed to prove some theorems which are associating with a vector x in K -dimensional real space. The co-ordinates of such a vector are x_1, x_2, \dots, x_k .

Theorem

Let ℓ , be a subset of R^k . Suppose that there is a constant C such that if $x \in \ell$, then $\sum_{i=1}^k X_i = C$

and $X_i \geq 0$ for $i = 1, 2, \dots, K$. If ℓ_i contains an element X^* such that

- i. $X_i^* > 0$ for $i = 1, 2, \dots, k$.
- ii. there are two distinct values among $X^*_1, X^*_2, \dots, X^*_k$
- iii. X^* minimized $\sum_{i=1}^k x_i^2$ over ℓ
- iv. X^* maximizes $\text{Max} \sum_{i=1}^k X_i$ over ℓ .

Proof of the Theorem is omitted because it is an extension to n -ary block designs cases from binary design. For the binary design cases proof is given in Cheng, and Bailey (1991).

Consider the criteria of the form $\sum_{i=1}^{V-1} (f\mu_{di})$, where f satisfies the conditions given in the above Theorem (5.5.1). The A and D criteria are covered by choosing $f(x) = x^{-1}$ and $-\log(x)$ respectively. Our most important interest i.e. E-Optimal criteria is covered as a point wise limit of criteria derived from functions satisfying the condition in the Theorem (5.5.1).

Theorem:

If $D(V,B,K)$ contains a connected PBNB (2) design d^* whose concurrence matrix is singular, then d^* is optimal over $D(V,B,K)$ with respect to any criterion of the form $\sum_{i=1}^{V-1} f(\mu_{di})$, where f satisfies the conditions given in Theorem (5.5.1). In particular, d^* is A, D and E-Optimal over $D(V,B,K)$.

Proof:

Let $K = V-1$, For $d \in D(V,B,K)$, put

$\mu_d = (\mu_{d1}, \mu_{d2}, \dots, \mu_{dk})$. Let $\ell = \{ \mu_d ; d \in D(V,B,K) \}$. For each $d \in D(V,B,K)$, we have

$$C_d = RI-K^{-1} N_d N_d' \quad \text{where } R = \frac{BK}{V}$$

Since d is n -ary, every diagonal entry of $C_d = \frac{RK - \Delta}{K}$ and so $\mu_{d1} + \mu_{d2} + \dots + \mu_{dk}$
 $= \text{tr}(C_d) = B(K-1)$.

Moreover, C_d has no negative eigenvalues. Thus ℓ satisfies the conditions of Theorem (5.5.1).

Let μ_1^* and μ_k^* be for μ_{d1}^* and μ_{dk}^* . Because d^* is connected, all $\mu_1^*, \mu_2^* \dots \mu_k^*$ are positive. Because d^* is PBNBD (2), there are two distinct values among $\mu_1^*, \mu_2^* \dots \mu_k^*$ [Connor and Cltworthy (1954) for binary, Soundarapandian (1980a) for n -ary designs].

The trace of C_{d^*} is equal to $\sum_{i=1}^k (\mu_{di}^*)^2$ and this is minimized [Cheng (1978)] in $D(V,B,K)$ in particular by d^* .

$$\text{We have } R \geq \max_{i=1}^k \mu_{di} = \mu_{d1}$$

If $N_d N_d'$ is singular, then C_d has atleast one eigenvalue equal to R . Hence μ_{d1}^* maximizes μ_{d1} over ℓ . Therefore, conditions (i), (ii), (iii) and (iv) of Theorem (5.51) are satisfied.

From Theorem (5.5.1), Theorem (5.5.2) is proved.

Corollary:

The dual of the design d^* in Theorem (5.5.2) is also optimal over $D(V,B,K)$ with respect to the same criteria.

Proof:

Let dual of d^* be d . Then we have $N_d N_d' = N_{d^*}' N_{d^*}$ which has the same non-zero eigenvalues as $N_{d^*}' N_{d^*}$. Since $N_{d^*}' N_{d^*}$ is singular and C_{d^*} has two distinct non-zero eigenvalues, it is clear that C_d has at most two distinct non-zero eigenvalues.

If C_d has only one non-zero eigenvalue, then the optimality of \bar{d} is obvious.

If C_d has two distinct non-zero eigen values, then $N_d N_d'$ must be singular.

Thus from Theorem (5.5.1) it is sufficient to show $\text{tr } c_d^2$ is minimized over $d \in D(V,B,K)$. Since $\text{tr}(N_d N_d') = \text{tr}(N_{d^*}' N_{d^*})^2$ and that d^* minimizes $\text{tr } c_d^2$ over $d \in D(V,B,K)$.

Hence proved.

VII. Applications

The above theorems and corollary can be utilized to establish the optimality of PBNB(2) designs of the following types.

- (i) All the PBNB designs with $\Lambda_2 = \Lambda_1 + a$ (a is a scalar) and $B < V$.
- (ii) All the resolvable PBIB (2) with $\Lambda_2 = \Lambda_1 \pm a$ and $B < V + K - 1$.
- (iii) All the singular group divisible designs with $\Lambda_2 = \Lambda_1 - 1$.
- (iv) All the semi-regular group divisible designs with $\Lambda_2 = \Lambda_1 + a$.

For various types of PBNBD (2), the reference may be made to the thesis of Soundarapandian (1981d). A Table of these types of balanced n-ary and partially balanced n-ary design are under preparation by Soundarapandian for publication.

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