INCOMPLETE BLOCK DESIGNS FOR GENERAL CORRELATION STRUCTURES

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This paper gives a combinatorial characterization of incomplete block designs for which the variance matrix of the generalized least squares estimate of treatment effects, under general within block correlation structures, is a constant multiple of that under the usual uncorrelated model. A familly of PBIB designs with the latter property is defined and some constructions are given. Efficiencies relative to universal optimality are evaluated for some examples and turn out to be satisfactory. In comparison to randomized block designs these are shown to perform better for highly corelated observations.

1. **Introduction.** Let $D(v.b.k)$ be the collection of all binary incomplete block designs in v treatments and b blocks each of size k. For d in $D(v,b,k)$ assume the usual linear model:

$$Y_d = T_d\alpha + B\beta + \epsilon \tag{1}$$

where $B = I_b \otimes 1_k$ is the $bk \times b$ plot-block imcidence matrix, T_d the $bk \times v$ plot-treatment incidence matrix, β the b-vector of fixed block effects, α the v-vector of treatments effects and ϵ the bk-vector of random errors such that:

$$E(\epsilon) = 0 \qquad Var(\epsilon) = \sigma_d^2(I_b \otimes V) \tag{2}$$

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where σ_d^2 is the variance of an observation and V the correlation matrix of any k observations within a block. Observations from different blocks are assumed to be uncorrelated. Let $\hat{\tau}$ be the generalized least squares estimate for the vector of corrected treatment effects $\tau_i = \alpha_i - \frac{1}{v}\Sigma_{j=1}^{v}\alpha_j$, $i = 1,\cdots,v$.

Martin and Eccleston (1991) have considered the structure of optimal incomplete block designs for a general V. In particular they considered designs which they have termed strongly directionally equineighboured (SDEN) and show that a (v,b,k)-SDEN is universally optimal (Kiefer 1975) for $\hat{\tau}$ over D(v,b,k) for any given correlation matrix V. As the authors pointed out, an SDEN with block size $k \geq 3$ is equivalent to a semi balanced array of strength 2 defined by Rao(1961,1973) and their results generalize earlier results on the optimality of these arrays by Morgan and Chakravarti (1988) and Cheng (1988).

An SDEN design d is such that the variance matrix of $\hat{\tau}$ under a general V is a constant multiple of that under the usual model with uncorrelated observations. In general designs with this property will be termed correlation-uniform.

A severe constraint on the existence of SDENs is that the number of blocks b must be a multiple of $v(v-1)/2$ if v is odd and a multiple of $v(v-1)$ if v is even, which results in an unconfortably large number of blocks; the object of this paper is to construct designs with smaller number of blocks than SDENs with equal number of treatments and discuss their performance for the estimation of treatment effects.

Section 2 gives a combinatorial characterization of correlation-uniform incomplete block designs with $k \geq 3$. In section 3 some PBIB designs which are also correlation-uniform are defined and called association-balanced designs (AB) and some constructions are given. In section 4 an approach similar to that in Gill and Shukla (1985) is used to assess the performance of AB designs relative to universal optimality. In section 5 some examples of AB designs are compared to a randomized complete block design with equal number of treatments and equal number of replications in the case of first order autoregressive correlation

Throughout the paper, designs are prefixed by a 3-tuple (v,b,k) where v is the number of treatments, b the number of blocks and k the block size. For the definitions of association scheme and PBIB designs, reference may be made to Raghavarao (1971).

2. Correlation-uniform designs. A binary incomplete (v,b,k) block design will be called pairwise uniform on the plots if it satisfies the following conditions :

c1: each treatment i, $i = 1,\cdots,v$, occurs equally often (r_i times) in each plot position ℓ, $\ell = 1,\cdots,k$.

c2: each unordered pair of treatments i,j, $i \neq j$, occurs equally often (λ_{ij} times) within the same block in each unordered pair of plot labels ℓ,ℓ', $\ell \neq \ell'$.

The numbers r_i's are the replcation parameters and λ_{ij}'s the index parameters.

Clearly, c2 implies c1 if $k \geq 3$.

EXAMPLE 1: (4,6,3) pairwise uniform design with $\lambda_{13} = \lambda_{14} = \lambda_{23} = \lambda_{24} = 1$ and $\lambda_{34} = 2$:

d_1

1	2	3	3	4	4
3	3	4	4	1	2
4	4	1	2	3	3

As in Kunert)1987), under (1) and (2), the information matrix of $\hat{\tau}$ for a given design d is:

$$C_d(V) = \sigma_d^{-2} \sum_{u=1}^{b} T'_{du} W(V) T_{du} \tag{3}$$

where $W(V) = V^{-1} - (1'_k V^{-1} 1_k)^{-1} V^{-1} 1_k 1'_k V^{-1}$, and T_{du} is the $k \times v$ plot-treatment incidence matrix for block u.

Correlaton-uniformity, defined earlier, calls for a design d such that:

$$C_d(V) = h(V) C_d(I) \qquad \text{for all positive definite V} \tag{4}$$

where h(V) is some constant.

The following lemma given by Chakravarti (1975) will be needed.

LEMMA 1. Let A be an $n \times n$ real matrix with non negative entries, $s_i > 0$ the sum of the entries in the *i-th* row of A, then if A is irreducible the matrix $Q = A - \mathrm{diag}(s_1,\cdots,s_n)$ must have rank $n - 1$.

THEOREM 1. A design in $D(v,b,k)$ with $k \geq 3$ is correlation-uniform if and only if it is pairwise uniform on the plots.

PROOF: Without loss of generality assume $\sigma_d^2 = 1$. Let d be pairwise uniform on the plots with replication parameters r_i, $i = 1,\cdots,v$ and index parameters λ_{ij}, $1 \leq i < j \leq v$. Simple algebraic computations give the entries of $C_d(V)$ as:

$$C_{d.ii}(V) = r_i \mathrm{tr}[W(V)] \quad i = 1,\cdots,v$$

$$C_{d.ji}(V) = C_{d.ij}(V) = \lambda_{ij} \sum_{1 \leq \ell < \ell' \leq k} w_{\ell\ell'} \quad 1 \leq i < j \leq v$$

where $w_{\ell\ell'}$ is the (ℓ,ℓ')-th entry of $W(V)$. Since $W(V)$ is symmetric with row and column sums equal to 0:

$$C_{d.ij}(V) = -\frac{\lambda_{ij}}{2}\mathrm{tr}[W(V)]$$

and $\mathrm{tr}[W(I)] = \mathrm{tr}(I_k - \frac{1}{k}1_k1'_k) = k-1$, so that:

$$C_d(V) = \frac{\mathrm{tr}[W(V)]}{k-1} C_d(I)$$

Conversely let d be a (v,b,k) correlation-uniform binary incomplete block design with R_i the total number of occurrences of treatment i, $r_{i\ell}$ the number of occurences of treatment i in plot label ℓ and $\lambda_{ij}^{\ell\ell'}$ the number of times the unordered pair of treatments i and j occurs within the same block in the unordered pair of plot labels ℓ and ℓ'. Then $C_d(V)$ has entries:

$$C_{d.ii}(V) = \sum_{\ell=1}^{k} r_{i\ell} w_{\ell\ell} \qquad i = 1,\cdots,v$$

$$C_{d.ij}(V) = \sum_{1 \leq \ell < \ell' \leq k} \lambda_{ij}^{\ell\ell'} w_{\ell\ell'} \qquad 1 \leq i \neq j \leq v$$

In particular, if $V = I$:

$$C_{d.ii}(I) = \frac{k-1}{k} R_i$$

$$C_{d.ij}(I) = -\frac{1}{k} \sum_{\ell < \ell'} \lambda_{ij}^{\ell\ell'}$$

equation (4) implies:

$$(5) \qquad \sum_{\ell=1}^{k} r_{i\ell} w_{\ell\ell} = \frac{k-1}{k} h(V) R_i \qquad i = 1,\cdots,v$$

(6) $$\sum_{\ell<\ell'} \lambda_{ii}^{\ell\ell'} w_{\ell\ell'} = -\frac{h(V)}{k} \sum_{\ell<\ell'} \lambda_{ij}^{\ell\ell'} \qquad 1 \le i \ne j \le v$$

summing equations (5) over i gives $h(V) = tr[W(V)]/(k-1)$.

Let $V(p,q)$ be the correlation matrix corresponding to the model where only observations within the same block in plot labels p and q are correlated with correlation coefficient ρ, all other observations being uncorrelated; and $\mathcal{V} = \{V(p,q): 1 \le p < q \le k\}$. Note that any matrix in $\mathcal{V}$ can be obtained from any other matrix in $\mathcal{V}$ by suitable pemutations of rows and columns. Some lengthy but straightforward algebraic computations show that the entries of the matrix $W(V(p,q))$, dentoted by $w_{\ell\ell'}(p,q)$ take the following 5 values:

$$x = w_{pp}(p,q) = w_{qq}(p,q) = \frac{1}{1-\rho^2} - \frac{2}{w(1+\rho)^2}$$

$$y = w_{\ell\ell}(p,q) = 1 - \frac{1}{w} \qquad \ell \notin \{p,q\}$$

$$a_0' = w_{pq}(p,q) = -\frac{\rho}{1-\rho^2} - \frac{2}{w(1+\rho)^2}$$

$$a_1' = w_{p\ell}(p,q) = w_{q\ell}(p,q) = -\frac{2}{w(1+\rho)} \qquad \ell \notin \{p,q\}$$

$$a_2' = w_{\ell\ell'}(p,q) = -\frac{1}{w} \qquad \{\ell,\ell'\} \cap \{p,q\} = \emptyset$$

where $w = 1_k'[V(p,q)]^{-1}1_k = (k-2) + \frac{2}{1+\rho}$

and $tr[W(V(p,q))] = 2x + (k-2)y = t$ say, is constant over $\mathcal{V}$.

Applying (6) for each element of $\mathcal{V}$, with $h(V) = t/(k-1)$, yields a system of $\binom{k}{2}$ linear equations:

$$a_1\Big\{\sum_{\ell \notin \{p,q\}} (\lambda_{ij}^{p\ell} + \lambda_{ij}^{q\ell})\Big\} + a_2\Big\{\sum_{\substack{\ell<\ell' \\ \{\ell,\ell'\}\cap\{p,q\}=\emptyset}} \lambda_{ij}^{\ell\ell'}\Big\} - a_0\lambda_{ij}^{pq} = 0 \qquad 1 \le p < q \le k$$

where $a_0 = -a_0' - \frac{t}{k(k-1)}$

$$a_i = a_i' + \frac{t}{k(k-1)} \qquad i = 1,2$$

Let $\gamma = (\lambda_{ij}^{12},\cdots,\lambda_{ij}^{1k},\lambda_{ij}^{23},\cdots,\lambda_{ij}^{k-1\ k})'$

The above equations may then be written in matrix form as:

$$(7) \qquad Q\gamma = 0$$

where Q is the square matrix of order $\binom{k}{2}$ given by:

$$Q = a_1 A_1 + a_2 A_2 - a_0 I$$

and A_i $i = 1,2$, are 0-1 matrices of order $\binom{k}{2}$ such that $A_1 + A_2 = J - I$, where J is the matrix with all entries equal to 1.

In the first part of the proof it has been shown that a vector γ with all entries equal is a solution to (7). To complete the proof it remains to show that the null space of Q has dimension 1 at least for some value of the correlation coefficient ρ.

Each row of Q sums to :

$$s(Q) = 2(k-2)a_1 + \frac{(k-2)(k-3)}{2}a_2 - a_0 = 0$$

So that each row of $A = a_1 A_1 + a_2 A_2$ sums to a_0, and for $\rho = \frac{1}{2}$:

$$a_0 = (k-2)(2k^2 - k + 1)/e \qquad a_1 = (k^2 - k + 2)/e \qquad a_2 = 2/e$$

where $e = k(k-1)(3k-2)$

For $k \geq 3$, $a_i > 0$, $i = 1,2$, so that A is irreducible with non negative entries, and lemma 1 implies that $\text{rank}(Q) = \binom{k}{2} - 1$.□

For block size $k = 2$, it is easily seen that (4) is satisfied for all d in $D(v,b,2)$.

3. Association-balanced designs. Given an association scheme in v symbols and s classes, a (v,b,k) binary incomplete block design will be said to be association-balanced (AB) if it satisfies the following conditions:

c3: each treatment occurs $r = b/v$ times in each plot label,

c4: each unordered pair of g-th associate symbols, $g = 1,\cdots,s$, occurs λ_g times within the same block in each unordered pair of plot labels.

Clearly, c3 and c4 are more restrictive conditions than c1 and c2 above and c4 implies c3 if $k \geq 3$; so that an AB design is correlation uniform. A (v,b,k)-AB design with index parameters $\lambda_1,\cdots,\lambda_s$ is also a (v,b,k) PBIB design with index parameters $\lambda_g\binom{k}{2}$ $g = 1,\cdots,s$, introduced by Bose and Nair (1939); and an SDEN design defined in Martin and Eccleston (1991) is also an AB design relative to the trivial association scheme with only one associate class.

EXAMPLE 2: (8,24,4) group divisible AB design with groups {1,5}, {2,6}, {3,7} and {4,8}, and index parameters $\lambda_1 = 0$ and $\lambda_2 = 1$:

d_2

1	5	2	6	3	7	4	8	1	5	2	6	3	7	4	8	1	5	2	6	3	7	4	8
2	6	5	1	4	8	7	3	3	7	8	4	5	1	2	6	4	8	3	7	6	2	5	1
3	7	8	4	5	1	2	6	4	8	3	7	6	2	5	1	2	6	5	1	4	8	7	3
4	8	3	7	6	2	5	1	2	6	5	1	4	8	7	3	3	7	8	4	5	1	2	6

The following theorem gives some series constructions af AB designs from known SDEN and PBIB designs, it is analogous to theorem 4.1 given by Chakravarti (1961) for the construction of partially balanced arrays.

THEOREM 2. The existence of an s associate class (v,b_0,q) PBIB design with index parameters $\gamma_1,\cdots,\gamma_s$ and an SDEN design in q treatments, block size k and index λ imply the existence of an s associate class (v,b,k) AB design where $b = \lambda b_0\binom{q}{2}$ and index parameters $\lambda_i = \lambda\gamma_i$, $i = 1,\cdots,s$.

PROOF: Block B_i $(i = 1,\cdots,b_0)$ of the PBIB design provide q symbols for an SDEN in $b_1 = \lambda\binom{q}{2}$ blocks $B_{i,1},\cdots,B_{i,b_1}$ each of size k. The set of blocks $B_{i,j}$, $i = 1,\cdots.b_0$ $j = 1,\cdots,b_1$, is clearly an AB design with the required parameters.

A review on constructions of PBIB designs is given in Raghavarao (1971), Clathworty (1973) gives an extensive list of these designs. The construction of (v,b,k) SDEN designs with index 1 and v an odd prime power is given by Rao (1961), where they are called orthogonal arrays of type 2 and strength 2, and later called semi balanced arrays in Rao (1973). The existence problem for v odd, index 1 and $k = 3,4,5$ have been settled by Mullin & al (1988), they show that a $(v,b,3)$ SDEN exists for all odd $v \geq 3$, a $(v,b,4)$ SDEN exists for all odd $v \geq 5$ (except possibly $v = 87$) and a $(v,b,5)$ SDEN exists for all odd $v \geq 5$ (except possibly $v \in \{33,39,51,87,219\}$).

Of special interest here is a two associate class AB design with index parameters λ_1 and λ_2 and smaller number of blocks than an SDEN with equal number of treatments and minimum number of blocks. These are such that $\lambda_i = 0$ for $i = 1$ or 2 if v is odd and $\lambda_i \leq 1$ for $i = 1$ or 2 if v is even. the following corollaries to the above theorem give some series constructions of these designs.

COROLLARY 1. The existence of an (m,b,k) SDEN design with index 1 implies the existence of :

(a) a group divisible $(mn,n^2m(m-1)/2,k)$ AB design where $m \leq n+1$, n prime or power of a prime, $\lambda_1 = 0$ and $\lambda_2 = 1$.

(b) a triangular $(m(m+1)/2,(m-1)m(m+1)/2,k)$ AB design with $\lambda_1 = 1$ and $\lambda_2 = 0$.

(c) an L_2-type $(m^2,m^2(m-1),k)$ AB design with $\lambda_1 = 1$ and $\lambda_2 = 0$.

PROOF : Theorems 8-5-7, 8-8-1 and 8-10-3 in Raghavarao (1971) respectively give the construction of a group divisible (mn,n^2,m), a triangular $(m(m+1)/2,m+1,m)$ and an L_2-type $(m^2,2m,m)$ PBIB design; application of theorem 2 to these PBIBDs and the SDEN gives the required AB designs.

COROLLARY 2. A triangular $(m(m+1)/2,(m-1)m(m+1)/2,3)$ AB design with $\lambda_1 = 1$ and $\lambda_2 = 0$ exists for any $m \geq 3$.

PROOF : Let the $\binom{m+1}{2}$ symbols of the triangular scheme be identified with the unordered pairs (i,j), $1 \leq i < j \leq m+1$, two pairs being first associates if they have one coordinate in common and second associate otherwise. The set of blocks $((i.j),(i,\ell),(j,\ell))$, $1 \leq i < j < \ell \leq m+1$, is an $(m(m+1)/2,b,3)$ PBIB design with index parameters $\gamma_1 = 1$ and $\gamma_2 = 0$, application of theorem 2 to this PBIB design and to a (3,3,3) SDEN gives the required AB design.□

Table 1 gives some parameter combinations of two associate class AB designs constructed by the above method.

TABLE 1

design label	v	b	k	λ_1	λ_2	association scheme
d_3	6	12	3	0	1	group divisible
d_4	10	30	3	1	0	triangular
d_5	9	18	3	1	0	L_2-type
d_6	9	27	3	0	1	group divisible
d_7	12	48	3	0	1	group divisible
d_8	15	60	5	1	0	triangular

If all observations are uncorrelated, it is well known that PBIB designs are partially variance balanced, in the sens that any two elementary treatment contrasts are estimated with the same variance if the corresponding pairs of treatments belong to the same associate class; since an AB design is a correlation uniform PBIB, it is indeed partially variance balanced for any positive definite correlation matrix V.

4. Efficiency relative to universal optimality. If a design d is connected, its information matrix $C_d(V)$ has exactly $v-1$ nonzero eigenvalues, let these be denoted by $\mu_{d,1} \geq \mu_{d,2} \geq \cdots \geq \mu_{d,v-1} > 0$. The universal optimality criteria defined by Kiefer (1975), calls for a design with maximum trace of $C_d(V)$ and all $\mu_{d,i}$'s equal. The A and D optimality criteria respectively call for the maximization of the functionnals:

$$\phi_A(d) = \frac{1}{v-1} \sum_{i=1}^{v-1} \mu_{d,i}^{-1} \qquad \phi_D(d) = \left(\prod_{i=1}^{v-1} \mu_{d,i}^{-1} \right)^{\frac{1}{v-1}}$$

Since $\mathrm{tr}(C_d) = b\mathrm{tr}(W)$ is constant over $D(v,b,k)$ define the A and D efficiencies of a design $d \in D(v,b,k)$, as in Gill and Shukla (1985), by:

$$e_A(d) = \frac{\phi_A(d^*)}{\phi_A(d)} \qquad e_D(d) = \frac{\phi_D(d^*)}{\phi_D(d)}$$

where d^* is a hypothetical universally optimal design whose information matrix $C_{d^*}(V)$ has nonzero eigenvalue $(\mu_{d,1} + \mu_{d,2} + \cdots + \mu_{d,v-1})/(v-1)$ with multiplicity $v-1$.

If d is correlation uniform both e_A and e_D are independant of V and attain their maximum value 1 for SDEN designs. Table 2 below give these efficiencies for some examples of designs mentionned earlier.

TABLE 2

design	e_A	e_D
d_1	0.818	0.908
d_2	0.980	0.989
d_3	0.961	0.980
d_4	0.947	0.973
d_5	0.888	0.942
d_6	0.969	0.983
d_7	0.975	0.986
d_8	0.942	0.972

The table shows all designs to be highly efficient.

5. Association-balance versus randomization. In this section, a (v,b,k) AB design is compared to a randomized complete block design with equal number of treatments v and equal number of replications $r = bk/v$, assuming a first order autoregressive (AR1) correlation matrix V with entries

$$v_{\ell\ell'} = \rho^{|\ell - \ell'|} \qquad 1 \leq \ell,\ell' \leq k$$

For the randomized complete block design, the variance of an elementary treatment contrast estimated by ordinary least squares is given, for example, in Williams (1952) as:

$$V_R = \frac{2\sigma_R^2}{r}(1 - \bar{\rho})$$

where σ_R^2 is the variance of an observation and $\bar{\rho}$ is the average correlation between observations from any two plots within a block taken over all possible randomizations. For AR1 correlation the expression of $\bar{\rho}$ (Williams 1952) is:

$$\bar{\rho} = \frac{2}{v(v-1)} \sum_{i=1}^{v-1} (v-i)\rho^i$$

Under (1) and (2), the average variance of an elementary treatment contrast estimated by generalized least squares for a designd d is (Kempthorne 1956):

$$V_d = 2(v-1)^{-1}\sigma_d^2 \sum_{i=1}^{v-1} \gamma_{d,i}^{-1}$$

where $\gamma_{d,i}$'s are the nonzero eigenvalues of $\sigma_d^2 C_d(V)$.

As in Gill and Shukla (1985), Williams (1952) and Morgan (1990), define the efficiency of a systematic design d relative to a randomized block design by $e_R = V_R/V_d$.

If d is an incomplete block design ($k < v$), it is intuitively clear that $\sigma_d^2 \leq \sigma_R^2$ because of the smaller block size. Hence assuming $\sigma_R^2/\sigma_d^2 = 1$ yields a lower bound to the true efficiency.

Table 3 below gives these efficiencies for four examples of AB designs d_2, d_3, d_4 and d_5 mentionned earlier, and for different values of ρ, assuming $\sigma_d^2/\sigma_R^2 = 1$. These are shown to perform better than the randomized complete block for highly correlated observations.

TABLE 3

ρ	d_2	d_3	d_4	d_5
−0.9	4.330	2.576	2.190	2.094
−0.8	2.224	1.442	1.234	1.182
−0.7	1.541	1.078	0.929	0.890
−0.6	1.216	0.909	0.788	0.755
−0.5	1.035	0.819	0.714	0.683
−0.4	0.928	0.770	0.676	0.646
−0.3	0.867	0.747	0.660	0.631
−0.2	0.836	0.741	0.661	0.630
−0.1	0.828	0.749	0.675	0.642
0.0	0.840	0.769	0.701	0.666
0.1	0.870	0.800	0.741	0.702
0.2	0.918	0.843	0.794	0.750
0.3	0.987	0.898	0.865	0.814
0.4	1.078	0.966	0.957	0.896
0.5	1.197	1.050	1.077	1.002
0.6	1.350	1.150	1.232	1.137
0.7	1.544	1.271	1.437	1.312
0.8	1.793	1.416	1.709	1.538
0.9	2.111	1.589	2.075	1.834

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