

## BLOCK DESIGNS FOR FIRST AND SECOND ORDER NEIGHBOR CORRELATIONS

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Constructions and optimality results are given for block designs under first and second order (NN1 and NN2, respectively) neighbor correlations, extending the work of Kiefer and Wynn. Conditions for optimality and minimality are given for the NN2 model and new minimality results are found for the NN1 case. Construction of NN2 optimum complete block designs is solved and combinatorial arrays are used for NN2 optimum incomplete block designs. In many cases these are minimum optimum NN1 designs as well. A new solution for block size 3 is given. A method for constructing NN1 designs with partial variance balance is introduced and several series of these designs are shown to enjoy weaker optimality properties.

**1. Introduction.** For a block design of  $b$  blocks with  $k$  plots per block, arbitrarily label the blocks  $1, \dots, b$  and the plots within a block  $1, \dots, k$ . Then each of the  $bk$  plots may be associated with one of the ordered pairs  $(l, s)$ ,  $l = 1, \dots, b$  and  $s = 1, \dots, k$ , with corresponding observation denoted  $Y_{l,s}$ . The numbering of the plots within a block may be thought of as an ordering of those plots, by which the  $j$ th-order nearest neighbor (NN $j$ ) covariance structure for the layout is given as

$$\text{cov}(Y_{l,s}, Y_{l',s'}) = \begin{cases} \sigma^2 \rho_{|s-s'|}, & l = l', |s - s'| \leq j, \\ 0, & \text{otherwise.} \end{cases}$$

To be considered here is the problem of allocation of a set of  $v$  treatments to the  $bk$  plots, assuming the usual additive model for block and treatment effects. The approach taken is that of Kiefer and Wynn (1981):

1. For the set of designs  $\chi$  under consideration, identify the class  $\chi^* \subset \chi$  which is optimum for uncorrelated errors.
2. Using least squares estimates, find the subclass  $\chi^{**} \subset \chi^*$  which is optimum for the appropriate covariance structure.

For one-way block designs with  $k$  plots per block, optimum classes  $\chi^*$  are, for  $k < v$  and  $k = v$ , the balanced incomplete block designs (BIBD) and the complete block designs, respectively [Kiefer (1958)]. Using the NN1 structure, Kiefer and Wynn (1981) found conditions for the classes  $\chi^{**}$  and illustrated a construction for the complete block case. Cheng (1983) gave several constructions for

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optimum BIBDs, including a graph theoretic algorithm for the case  $k = 3$  and construction by development of ordinary BIBDs according to optimum complete block designs. Here, the optimality results of Kiefer and Wynn (1981) are extended to the  $NN2$  case, and a solution is given for  $NN2$  optimum complete block designs.  $NN1$  and  $NN2$  optimality conditions are shown to be identical for  $k = 3$ , and another (simpler) solution is given for this case based on combinatorial arrays. More generally, transitive and semibalanced arrays provide a large number of  $NN2$  optimum designs. Of special interest is that in many cases  $NN2$  optimality can be had in the same number of blocks as  $NN1$  optimality.

Kiefer and Wynn (1981) also proposed the use of "equineighbored" BIBDs (EBIBDs), a class of designs which do not necessarily satisfy the strong optimality conditions for the  $NN1$  case. Here another approach is introduced, analogous to the use of partially balanced incomplete block designs (PBIBDs) in the presence of uncorrelated errors, producing a number of designs which enjoy weaker optimality properties. In particular, Type II optimality is considered. A design is Type II optimum if it minimizes the maximum variance of estimated elementary treatment contrasts [Takeuchi (1961)].

We wish to emphasize that the estimation procedure used here is that of least squares. We refer the reader to Kiefer and Wynn [(1981), pages 738–741] for detailed justification and explanation of this approach and note especially their conclusion that "in an approximate sense we are justified in using the ordinary least squares estimate if we feel that any autocorrelation present is small." In extending their work to the  $NN2$  case, it is worth pointing out that in practice we usually expect  $\rho_2$  to be the smaller of the two correlations, say  $\rho_2 = \alpha\rho_1$ , where  $0 \leq \alpha \leq 1$ , so that by their arguments the approach is valid for the  $NN2$  model whenever it is for the  $NN1$  model. Even if one suspects  $\alpha \approx 0$ , the  $NN2$  optimum designs are still  $NN1$  optimum and hence may be thought of as providing protection against an "unexpected" correlation. In those cases where the two models require the same number of blocks, the  $NN2$  optimum designs are to be preferred.

As an alternate approach to block designs with correlated plots, employing weighted least squares and a different correlation model, we refer the reader to Kunert (1985a).

Many of the results obtained here employ certain decompositions of graphs. A brief listing of needed concepts and results from graph theory is given next [see Berge (1973)].

A graph  $G = G(E, V)$  consists of a set  $V$  of elements called vertices and a collection  $E$  of unordered pairs of elements of  $V$  called edges. An edge  $(i, j) \in E$  is said to be incident with the vertices  $i$  and  $j$ ;  $i$  and  $j$  are adjacent vertices.

A path in a graph is an alternating sequence of vertices and edges, beginning and ending with vertices, such that no vertex is repeated and such that every edge is incident with the vertices immediately preceding and succeeding it. The number of edges in a path is its length. Clearly, a path of length  $l$  may be denoted by the appropriate sequence of  $l + 1$  vertices. A cycle is a closed path, that is, a path for which the initial and final vertices are the same. A Hamiltonian cycle in  $G$  is a cycle that includes every vertex in  $G$ . A Hamiltonian cycle

decomposition of  $G$  is a set of Hamiltonian cycles in  $G$  that collectively include every edge of  $G$ , but for which no two of the cycles contain a common edge.

A graph is complete if the edges are each of the unordered pairs of distinct vertices from  $V$  exactly once. For  $|V| = v$ , this graph will be denoted  $K_v$ .  $K_v^2$  will be used to denote the graph with  $v$  vertices and two edges connecting each pair of vertices. There is a Hamiltonian cycle decomposition of  $K_v$  if  $v$  is odd and for  $K_v^2$  for all  $v$ .

**2. Optimality results.** The notation developed here follows that of Kiefer and Wynn (1981). With the established labeling (and hence ordering) of plots within a block, call plots 1 and  $k$  end plots and plots 2 and  $k - 1$  next-to-end plots. For a binary block design, let  $A_i$  equal the set of blocks containing treatment  $i$ ; let  $e_i$  equal the number of blocks for which treatment  $i$  occurs on an end plot; let  $f_i$  equal the number of blocks for which treatment  $i$  occurs on a next-to-end plot; let  $e_{ij}$  equal the number of blocks containing both  $i$  and  $j$  for which at least one of  $i$  and  $j$  is on an end plot, where a block is counted twice if both  $i$  and  $j$  are on an end plot; let  $f_{ij}$  equal the number of blocks containing both  $i$  and  $j$  for which at least one of  $i$  and  $j$  is on a next-to-end plot, where a block is counted twice if both  $i$  and  $j$  are on a next-to-end plot; and let  $N_{ij}^t$  equal the number of blocks in which  $i$  and  $j$  occur as  $t$ th neighbors, that is, are separated by  $t - 1$  plots ( $i \neq j$ ).

For a BIBD with  $b$  blocks,  $v$  treatments,  $k$  plots per block,  $r$  replicates and treatment concurrence number  $\lambda$ , we have the following relationships among these quantities (used without further mention in many of the proofs):

$$\begin{aligned} \sum_{j \neq i} N_{ij}^1 &= 2r - e_i, & \sum_{j \neq i} N_{ij}^2 &= 2r - e_i - f_i, \\ \sum_{j \neq i} e_{ij} &= (k - 2)e_i + 2r, & \sum_{j \neq i} f_{ij} &= (k - 2)f_i + 2r, \\ \sum_i e_i &= 2b \quad \text{and for } k > 3, & \sum_i f_i &= 2b. \end{aligned}$$

The expected value of an observation is taken to be additive in the block and treatment effects:  $E(Y_{l,s}) = \mu + \beta_l + \alpha_{(l,s)}$ , where  $\alpha_{(l,s)}$  is the effect of the treatment allocated to plot  $(l, s)$ . Least squares analysis of a BIBD yields  $I^T \hat{t}$  as the best linear unbiased estimator (BLUE) of the contrast  $I^T \alpha$ , where  $\hat{t}_i = k(\lambda v)^{-1} Q_i$  and the  $Q_i$ 's are the adjusted treatment totals. Employing the results (5.1) and (5.2) of Kiefer and Wynn [(1981), page 748] gives

**LEMMA 2.1.** *Let  $\hat{t}_i$  be as previously defined and suppose the NN2 covariance structure holds. If  $k \geq 4$ ,*

$$\begin{aligned} \text{var}(\hat{t}_i) &= \sigma^2(\lambda v)^{-2} \{ r [ k(k - 1) - 2(k + 1)\rho_1 - 2(k + 2)\rho_2 ] \\ &\quad + 2k(\rho_1 + \rho_2)e_i + 2k\rho_2 f_i \}, \\ \text{cov}(\hat{t}_i, \hat{t}_j) &= \sigma^2(\lambda v)^{-2} \{ -\lambda [ k + 2(k + 1)\rho_1 + 2(k + 2)\rho_2 ] \\ &\quad + k\rho_1 (kN_{ij}^1 + e_{ij}) + k\rho_2 (kN_{ij}^2 + e_{ij} + f_{ij}) \}. \end{aligned}$$

If  $k = 3$ ,

$$\begin{aligned}\text{var}(\hat{t}_i) &= 2\sigma^2(\lambda v)^{-2}[r(3 - 4\rho_1 + \rho_2) + 3e_i(\rho_1 - \rho_2)], \\ \text{cov}(\hat{t}_i, \hat{t}_j) &= \sigma^2(\lambda v)^{-2}[6(\rho_1 - \rho_2)N_{ij}^1 - \lambda(3 + 2\rho_1 - 5\rho_2)].\end{aligned}$$

Optimality conditions may now be found by employing Kiefer and Wynn's (1981) analogue of the well known result of Kiefer (1975): Obtain complete symmetry of the covariance matrix and minimize the trace [for discussion of this sense of optimality, called weakly universal optimality, see Kiefer and Wynn (1981)].

**THEOREM 2.1.** *A BIBD is weakly universally optimum among the BIBDs with the same values of  $v$ ,  $b$  and  $k$  for the NN2 covariance structure if*

- (i) *the quantities  $kN_{ij}^1 + e_{ij}$  are all equal ( $i \neq j$ );*
- (ii) *the quantities  $kN_{ij}^2 + e_{ij} + f_{ij}$  are all equal ( $i \neq j$ ).*

For  $k = 3$ , conditions (i) and (ii) are equivalent to equality of the  $N_{ij}^1$  ( $i \neq j$ ).

**PROOF.** Lemma 2.1 shows that the stated conditions give equality of the off-diagonal elements, and hence equality of the diagonal elements, since in the covariance matrix all row sums are zero. That all competitors have the same trace follows also from Lemma 2.1 upon noting that  $\sum_i e_i = \sum_i f_i = 2b$ .

For  $k = 3$ , Lemma 2.1 shows that equality of the  $N_{ij}^1$  yields optimality. Equivalence with the conditions of the theorem follows since for  $k = 3$ ,  $N_{ij}^1 + N_{ij}^2 = \lambda$ ,  $f_{ij} = N_{ij}^1$  and  $N_{ij}^1 + e_{ij} = 2\lambda$ .  $\square$

Following the same proof with  $\rho_2 = 0$  gives the NN1 result.

**COROLLARY 2.1** (Kiefer and Wynn). *A BIBD is weakly universally optimum among the BIBDs with the same values of  $v$ ,  $b$  and  $k$  for the NN1 covariance structure if the quantities  $kN_{ij}^1 + e_{ij}$  are all equal ( $i \neq j$ ).*

A BIBD which satisfies the conditions of Theorem 2.1 is said to be NN2 optimum or simply a NN2 BIBD. Likewise a BIBD satisfying Corollary 2.1 is said to be NN1 optimum or a NN1 BIBD. For given  $v$  and  $k$ , a design is said to be minimum if it has the smallest possible  $b$  satisfying the appropriate conditions. The next two results aid in establishing minimality of NN1 and NN2 optimum designs.

**THEOREM 2.2.** (i) *A NN1 BIBD satisfies  $k|4\lambda$ . If  $k \not\equiv 0 \pmod{4}$  or if  $v \equiv 2$  or  $3 \pmod{4}$ , then  $k|2\lambda$ .*

(ii) *A NN2 BIBD satisfies  $k(k-1)|4\lambda$ . If  $k \not\equiv 0 \pmod{4}$  or if  $v \equiv 2$  or  $3 \pmod{4}$ , then  $k(k-1)|2\lambda$ .*

**PROOF.** The results are immediate upon summing each of the quantities  $kN_{ij}^1 + e_{ij}$  and  $kN_{ij}^2 + e_{ij} + f_{ij}$  over  $i$  and  $j$  and dividing by  $v(v - 1)$ .  $\square$

**THEOREM 2.3.** *A NN1 BIBD for which  $2\lambda \not\equiv 0 \pmod{k}$  satisfies  $8(r - \lambda) \geq k^2$ .*

**PROOF.**

$$\begin{aligned} \sum_i \sum_{j \neq i} N_{ij}^1 &= \sum_i (2r - e_i) = 2vr - 2b = 2\lambda v(v - 1)/k \\ &\Rightarrow \sum_i \sum_{j \neq i} N_{ij}^1/v(v - 1) = 2\lambda/k \\ &\Rightarrow \text{the } N_{ij}^1 \text{ are not all equal, since } k \nmid 2\lambda. \end{aligned}$$

Hence  $\exists i', j'$  such that

$$N_{i',j'}^1 \leq \text{int}(2\lambda/k) = (4\lambda - k)/2k$$

$$\Rightarrow e_{i',j'} = 2\lambda + 4\lambda/k - kN_{i',j'}^1 \geq 2\lambda + 4\lambda/k - (4\lambda - k)/2 = (8\lambda + k^2)/2k.$$

But equality of the

$$kN_{ij}^1 + e_{ij} \Rightarrow \text{equality of the } e_i \Rightarrow 4b/v = e_{i'} + e_{j'} \geq e_{i',j'} \geq (8\lambda + k^2)/2k$$

and the desired inequality follows.  $\square$

The results for complete block designs are derived in a similar fashion and are stated together as the final result of this section.

**THEOREM 2.4.** *A complete block design with  $v$  treatments arranged in  $b$  blocks is NN2 optimum if*

- (i) *the  $N_{ij}^1$  are all equal ( $i \neq j$ );*
- (ii) *the  $N_{ij}^2$  are all equal ( $i \neq j$ ).*

*The conditions imply that  $v(v - 1) \mid 2b$ .*

**3. Complete block designs.** Denote by  $B_v$  the  $v \times v$  array with  $i, j$  entry

$$\left( i + (-1)^{j+1} \text{int} \left( \frac{j+1}{2} \right) \right) \pmod{v}, \quad i = 0, 1, \dots, v - 1, \quad j = 0, 1, \dots, v - 1.$$

For even  $v$ , let  $D_v$  be the  $v/2 \times v$  array given by the first  $v/2$  rows of  $B_v$ . Considering the rows of the arrays as ordered blocks, it is well known that

$$\begin{aligned} N_{ij}^1 &= 2, & i \neq j \text{ for } B_v, \\ N_{ij}^1 &= 1, & i \neq j \text{ for } D_v, \end{aligned}$$

so they are minimum optimum complete block designs for the NN1 structure [compare Theorem 4.2 of Kiefer and Wynn (1981)].

LEMMA 3.1. For  $B_v$ , with rows as ordered blocks,

$$N_{ij}^2 = v - 2, \quad i - j \equiv \pm 1 \pmod{v},$$

$$= 0, \quad \text{otherwise.}$$

For  $D_v$ , with rows as ordered blocks,

$$N_{ij}^2 = (v - 2)/2, \quad i - j \equiv \pm 1 \pmod{v},$$

$$= 0, \quad \text{otherwise.}$$

The condition  $i - j \equiv \pm 1 \pmod{v}$  of the lemma simply says that  $i$  and  $j$  are adjacent in the first column of  $B_v$  when that column is considered as a cycle.

THEOREM 3.1. There is a complete block design in  $b = v(v - 1)/2$  blocks for which the  $N_{ij}^1$  are all equal ( $i \neq j$ ) and the  $N_{ij}^2$  are all equal ( $i \neq j$ ) and thus a minimum optimum complete block design for the NN2 structure.

PROOF. CASE (i).  $v$  is odd. Let  $c_1, c_2, \dots, c_{(v-1)/2}$  be any Hamiltonian cycle decomposition of  $K_v$ . Form a path  $p_i$  from  $c_i$  by arbitrarily deleting any one edge and define a permutation  $f_i$  on  $\{0, 1, \dots, v - 1\}$  by the map of the first column of  $B_v$  onto  $p_i$ , i.e.,  $f_i(j) = p_{ij}$ , where  $p_i = (p_{i0}, p_{i1}, \dots, p_{i, v-1})$ . Since each pair of symbols is adjacent in exactly one of the  $c_i$ , the required design is given by the rows of the arrays

$$f_1(B_v), f_2(B_v), \dots, f_{(v-1)/2}(B_v)$$

by virtue of Lemma 3.1 and the comment immediately following it.

CASE (ii).  $v$  is even. Proceed as in case (i) using any Hamiltonian cycle decomposition of  $K_v^2$  to obtain  $v - 1$  permutations of the initial  $v/2$  blocks of  $D_v$ . □

EXAMPLE 1. NN2 optimum complete block design with  $v = 6$  treatments:

$B_6$							
0	1	5	2	4	3	$D_6$	$p_1 = (5, 3, 2, 4, 1, 0)$
1	2	0	3	5	4		$p_2 = (5, 4, 3, 0, 2, 1)$
2	3	1	4	0	5		$p_3 = (5, 0, 4, 1, 3, 2)$
3	4	2	5	1	0		$p_4 = (5, 1, 0, 2, 4, 3)$
4	5	3	0	2	1		$p_5 = (5, 2, 1, 3, 0, 4)$
5	0	4	1	3	2		

The rows of the following five arrays form the blocks of the design:

$f_1(D_6)$	$f_2(D_6)$	$f_3(D_6)$	$f_4(D_6)$	$f_5(D_6)$
5 3 0 2 1 4	5 4 1 3 2 0	5 0 2 4 3 1	5 1 3 0 4 2	5 2 4 1 0 3
3 2 5 4 0 1	4 3 5 0 1 2	0 4 5 1 2 3	1 0 5 2 3 4	2 1 5 3 4 0
2 4 3 1 5 0	3 0 4 2 5 1	4 1 0 3 5 2	0 2 1 4 5 3	1 3 2 0 5 4

4. Incomplete block designs. In this section combinatorial arrays will be used to construct optimal designs.

A  $t \times N$  array of  $v$  symbols is said to be semibalanced of strength  $d$  and index  $l = N/\binom{v}{d}$  if for any choice of  $d$  rows, the  $N$  columns contain each of the  $\binom{v}{d}$

unordered  $d$ -tuples of distinct symbols exactly  $l$  times. Such an array will be denoted  $SB(N, t, v, d)$ . A transitive array,  $TA(N, t, v, d)$  of strength  $d$  and index  $l = (v - d)!N/v!$  is a  $t \times N$  array of  $v$  symbols such that for any choice of  $d$  rows, the  $N$  columns contain each of the  $v!/(v - d)!$  ordered  $d$ -tuples of distinct symbols exactly  $l$  times. Clearly a transitive array of strength  $d$  and index  $l$  is a semibalanced array of strength  $d$  and index  $l(d!)$ . Transitive arrays have been treated by a number of authors, especially for their relationship to sets of mutually orthogonal Latin squares [e.g. Bose, Shrikhande and Parker (1960)]. Important here will be that a set of  $t - 1$  mutually orthogonal Latin squares of order  $v$  implies the existence of  $TA(v(v - 1), t, v, 2)$ . Semibalanced arrays have been investigated by Rao (1961). Ramanujacharyulu (1966) and Mukhopadhyay (1978) who has given the strongest results. Both semibalanced and transitive arrays provide convenient constructions of  $NN2$  optimum designs.

**THEOREM 4.1.** *The existence of a semibalanced array  $SB(lv(v - 1)/2, k, v, 2)$  implies the existence of a  $NN2$  optimum BIBD with parameters  $v, k$  and  $b = lv(v - 1)/2$ .*

**PROOF.** Taking the columns of the array as ordered blocks, it is easy to see that the indicated BIBD is obtained. Also,  $N_{ij}^1 = l(k - 1)$ ,  $N_{ij}^2 = l(k - 2)$ ,  $e_{ij} = 2l(k - 1)$  and  $f_{ij} = 2l$  for  $k = 3$ ,  $f_{ij} = e_{ij}$  for  $k > 3$ .  $\square$

Although not needed here, it may be shown that semibalanced arrays are optimum for an arbitrary  $NNj$  correlation model. For details in the context of generalized Youden designs, see Kunert (1985b).

**COROLLARY 4.1.** *Each of the following conditions is sufficient for  $SB(v(v - 1)/2, k, v, 2)$  to be a minimum  $NN2$  BIBD:*

- (i)  $k \not\equiv 0 \pmod{4}$ .
- (ii)  $k \equiv 0 \pmod{4}$  and either  $k > \frac{2}{3}v$  or  $v \equiv 2$  or  $3 \pmod{4}$ .
- (iii)  $k = 4$ .

**PROOF.** (i) follows from Theorem 2.2 and (ii) from Theorems 2.2 and 2.3. To show (iii), it will be shown that  $k = 4, \lambda = 3$  is impossible under  $NN1$  conditions. With  $k = 4$ , a pair of treatments may occur in four distinct orientations  $\alpha, \beta, \gamma$  and  $\delta$  with respective contributions of 5, 1, 2 and 4 to  $kN_{ij}^1 + e_{ij}$ :

$$\begin{array}{cccc} \underline{\alpha} & \underline{\beta} & \underline{\gamma} & \underline{\delta} \\ \left| \begin{array}{c} i \\ j \\ - \\ - \end{array} \right| & \left| \begin{array}{c} i \\ - \\ j \\ - \end{array} \right| & \left| \begin{array}{c} i \\ - \\ - \\ j \end{array} \right| & \left| \begin{array}{c} - \\ i \\ j \\ - \end{array} \right| \end{array}$$

If  $\lambda = 3$ ,  $NN1$  optimality implies  $kN_{ij}^1 + e_{ij} = 9$ , so  $i$  and  $j$  must have either orientations  $\alpha, \gamma, \gamma$  or  $\beta, \delta, \delta$ . Counting over all possible pairs of treatments,

$2\binom{v}{2} = v(v-1)$   $\gamma$  and  $\delta$  orientations are required, but only  $2b = v(v-1)/2$  are available.  $\square$

The next result gives conditions for semibalanced arrays to be NN1 as well as NN2 minimum optimum. For integers  $x$  and  $y$ , define  $(x, y)$  equal to the greatest common divisor of  $x$  and  $y$ .

**THEOREM 4.2.** (i) *If  $k$  is odd, (a)  $(k-1, v-1) = 2 \Rightarrow \text{SB}(v(v-1)/2, k, v, 2)$  is minimum optimum for the NN1 and NN2 models; (b)  $(k-1, v-1) = 1 \Rightarrow \text{SB}(v(v-1), k, v, 2)$  is minimum optimum for the NN1 and NN2 models.*

(ii) *If  $k \equiv 2 \pmod{4}$  and  $(k-1, v-1) = 1$ , then  $\text{SB}(v(v-1)/2, k, v, 2)$  is minimum optimum for the NN1 and NN2 models.*

(iii) *If  $(k(k-1), v(v-1)) = 2$ , then  $\text{SB}(v(v-1)/2, k, v, 2)$  is minimum optimum for the NN1 and NN2 models.*

**PROOF.** For any BIBD,  $r = \lambda(v-1)/(k-1) \Rightarrow (k-1)|(k-1, v-1)\lambda$ . From Theorem 2.2(i), if  $k$  is odd, then  $k|\lambda \Rightarrow k(k-1)|(k-1, v-1)\lambda$ . Likewise

$$k \equiv 2 \pmod{4} \Rightarrow k|2\lambda \Rightarrow k(k-1)|(k-1, v-1)2\lambda.$$

In general,  $b = \lambda v(v-1)/k(k-1)$  and  $(k(k-1), v(v-1)) = 2 \Rightarrow v(v-1)|2b$ .  $\square$

A few of the many possible corollaries are listed next.

**COROLLARY 4.2.** *If  $k-1$  is a power of 2 and  $v$  is even,  $\text{SB}(v(v-1), k, v, 2)$  is minimum optimum for the NN1 and NN2 models whenever it exists.*

**EXAMPLE 2.** Setting  $k = 5$  in Corollary 4.2,  $\text{TA}(v(v-1), 5, v, 2)$  exists for any even  $v$  for which there are at least four mutually orthogonal Latin squares of order  $v$ . Included for  $v \leq 100$  are  $v = 8, 12, 16, 32, 40, 50, 54, 56$  and  $v = 2s$ ,  $s = 32, 33, \dots, 50$  [see Raghavarao (1971)].

**COROLLARY 4.3.** *If  $v = 2^n$  and  $v-1$  is prime,  $\text{TA}(v(v-1), k, v, 2)$  is minimum optimum for the NN1 and NN2 models for  $k = 4t-1$ ,  $t = 1, 2, \dots, 2^{n-2} - 1$ .*

**EXAMPLE 3.**  $v = 32$  in Corollary 4.3 yields the minimum optimum designs with  $k = 3, 7, 11, 15, 19, 23$  and  $27$ .

**COROLLARY 4.4.** *If  $k-1$  is a power of 2 and  $v \equiv 3 \pmod{4}$ , then  $\text{SB}(v(v-1)/2, k, v, 2)$  is minimum optimum for the NN1 and NN2 models whenever it exists.*

**EXAMPLE 4.** For  $k = 5$ , arrays satisfying Corollary 4.4 can be constructed by (4.1) for  $v \equiv 7, 19, 23, 43, 47$  and  $59 \pmod{60}$ .



The case  $k = 3$  can also be solved by array constructions. If  $v$  is odd, an  $NN1/NN2$  design must have a multiple of  $v(v - 1)/2$  blocks. The results of Mukhopadhyay (1978) imply the existence of the appropriate semibalanced arrays, but it is simpler to take the columns of the array [Gassner (1965)]:

$$(4.1) \quad \begin{aligned} &\text{place } (i + rj) \pmod{v} \text{ in row } r, \text{ column } \frac{i(v - 1)}{2} + j, \\ &r = 0, 1, 2; i = 0, 1, \dots, v - 1; j = 1, 2, \dots, \frac{(v - 1)}{2}, \end{aligned}$$

which is also semibalanced. (In fact,  $r$  may range up to one less than the smallest prime divisor of  $v$ .)

For  $k = 3$  and even  $v$ , a minimum of  $v(v - 1)$  blocks is required [Theorem 4.2(i)]. Hence a three rowed transitive array of strength 2 will suffice.

**THEOREM 4.3.** *Let  $v \geq 4$  be an integer and form a  $3 \times v(v - 1)$  array as follows. For  $i = 0, 1, \dots, v - 1$  and  $j = 1, 2, \dots, v - 1$  put  $i$  in column  $i(v - 1) + j$  of row 1 and put  $(i + j) \pmod{v}$  in column  $i(v - 1) + j$  of row 2. For row 3, for  $t = 1, 2, \dots, v - 2$ , put  $(t + l) \pmod{v}$  in column*

$$\begin{aligned} &(l - 1)(v - 1) + t - l + 1, \quad l = 1, 2, \dots, t, \\ &l(v - 1) + t - l + v, \quad l = t + 1, \dots, v - 1. \end{aligned}$$

*Also, put 1 in column  $v - 1$  and put  $v - 2$  in column  $(v - 1)^2 + 1$ . Finally, for  $i = 1, \dots, (v - 4)/2$  put*

$$\begin{aligned} &2i \pmod{v} \quad \text{in column } i(v - 2) + v, \\ &2i + 1 \pmod{v} \quad \text{in column } i(v - 2) + v - 1 \end{aligned}$$

*and for  $i = (v - 2)/2, \dots, v - 2$ , put*

$$\begin{aligned} &2i \pmod{v} \quad \text{in column } i(v - 2) + v - 1, \\ &2i + 1 \pmod{v} \quad \text{in column } i(v - 2) + v. \end{aligned}$$

*The array is  $TA(v(v - 1), 3, v, 2)$ .*

**PROOF.** The array is discussed in Morgan (1984).  $\square$

**EXAMPLE 5.**  $v = 6$  in Theorem 4.3 gives  $TA(30, 3, 6, 2)$ :

0 0 0 0 0	1 1 1 1 1	2 2 2 2 2	3 3 3 3 3	4 4 4 4 4	5 5 5 5 5
1 2 3 4 5	2 3 4 5 0	3 4 5 0 1	4 5 0 1 2	5 0 1 2 3	0 1 2 3 4
2 3 4 5 1	4 5 0 3 2	0 1 4 5 3	2 0 1 4 5	2 3 5 0 1	4 0 1 2 3

Two  $NN1$  or  $NN2$  optimum designs may be said to be equivalent if they can be made identical by relabeling of blocks and treatments and by reversing the order of blocks. This leads to a characterization of the minimum optimum BIBDs for  $k = 3$ .

**THEOREM 4.4.** *A NN1/NN2 minimum optimum BIBD with  $k = 3$  is equivalent to a semibalanced array.*

**PROOF.** The result will be proven for even  $v$ , the similar proof for odd  $v$  being even simpler. With  $v$  even, the minimum optimum design must have  $b = v(v - 1)$ ,  $\lambda = 6$ ,  $N_{ij}^1 = 4$  and  $N_{ij}^2 = 2$  for all  $i \neq j$ . Arrange the blocks side to side in any order to form a  $3 \times v(v - 1)$  array, arbitrarily orienting each block (e.g., the block  $\begin{smallmatrix} a & \\ b & \end{smallmatrix}$  may also be taken as  $\begin{smallmatrix} c & \\ b & \end{smallmatrix}$ , one orientation being the reverse of the other). For any column of the array, call the pair formed by rows 1 and 2 an upper pair and the pair formed by rows 2 and 3 a lower pair. Let  $N_{ij}^{1u}$  be the number of times symbols  $i$  and  $j$  occur as an upper pair and let

$$U = \# \{ (i, j) : i < j \text{ and } N_{ij}^{1u} = 3 \} + 2 \times \# \{ (i, j) : i < j \text{ and } N_{ij}^{1u} = 4 \}.$$

If  $U = 0$ , the array is semibalanced. Suppose  $U > 0$ ; it will be shown that  $U$  can always be reduced by 1.

Choose any pair  $i, j$  such that  $N_{ij}^{1u} > 2$  and reverse one of the columns in which  $i$  and  $j$  occur as an upper pair. Either  $U$  is reduced by 1 or  $N_{i'j'}^{1u}$  is increased by 1 to 3 or 4 for some pair  $i', j'$ , in which case  $U$  is unchanged. In the latter case, choose another column in which  $i'$  and  $j'$  occur as an upper pair and reverse it. Again either  $U$  is reduced or  $N_{i''j''}^{1u}$  is increased by 1 to 3 or 4 for some pair  $i'', j''$ . If again the latter occurs, choose another column in which  $i''$  and  $j''$  occur as an upper pair and reverse it, being sure not to reverse any previously reversed column. Continue reversing columns in this manner, subject to the constraint that no column is reversed more than once, until either  $U$  is reduced by 1 or no column is available for reversing. It will now be shown that the second possibility cannot occur.

Suppose the algorithm stops without reducing  $U$ . Let  $c_1$  be the last column reversed and let  $i, j$  be the upper pair of  $c_1$ . Then  $N_{ij}^{1u} > 2$  and there are  $s \geq 2$  other columns containing  $i, j$  as an upper pair which by assumption have all been previously reversed. Since the algorithm did not stop upon reversal of any of these  $s$  columns, there are  $s$  corresponding columns for which  $i, j$  is a lower pair. Hence there are at least  $2s + 1 \geq 5$  columns containing  $i$  and  $j$  as first neighbors, which contradicts  $N_{ij}^1 = 4$ .  $\square$

That a minimum NN1 BIBD with  $k = 3$  and even  $v$  need not be equivalent to a transitive array is shown by Example 6.

**EXAMPLE 6.**

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

By Theorem 4.4, this array is equivalent to a semibalanced array. But column reversals cannot give transitivity with respect to the pair (1, 2).

**5. Partially variance balanced designs.** By developing an ordinary BIBD according to the blocks of a  $NN1$  optimum complete block design on  $k$  treatments, Cheng (1983) obtained the following construction technique for  $NN1$  BIBDs.

**THEOREM 5.1.** *The existence of a BIBD  $D_0$  with parameters  $v_0$ ,  $k_0 = k$  and  $\lambda_0$  implies the existence of a  $NN1$  BIBD with parameters  $v = v_0$ ,  $k$  and  $\lambda = \lambda_0 k/2$  or  $\lambda_0 k$ , where the value of  $\lambda$  is for even or odd  $k$ , respectively. The developed design is minimum optimum if any one of the following conditions holds:*

- (i)  $\lambda_0 = (k - 1)/(k - 1, v - 1)$  and either  $k \not\equiv 0 \pmod{4}$  or  $v \equiv 2$  or  $3 \pmod{4}$ .
- (ii)  $k \equiv 0 \pmod{4}$ ,  $\lambda_0 = k - 1$ ,  $(k - 1, v - 1) = 1$  and  $k > \frac{2}{3}v$ .
- (iii)  $\lambda_0 = 1$ .

The minimality conditions (i)–(iii), which follow from Theorems 2.2(i) and 2.3, may be used to sharpen some of the results of Cheng [(1983); see his Theorem 3.3 and Corollary 4.5].

In this section, a different development technique is proposed, producing designs in fewer blocks at the expense of sacrificing the complete symmetry of  $\text{var}(\hat{t})$ . These designs may be compared to the EBIBDs of Kiefer and Wynn (1981): BIBDs with equality of the  $N_{ij}^1$ , which when not  $NN1$  optimum (i.e.,  $e_{ij}$  all equal as well) also lose complete symmetry of  $\text{var}(\hat{t})$ . For EBIBDs, the number of distinct variances for estimation of elementary treatment contrasts equals the number of distinct  $e_{ij}$ 's with the range of these variances proportional to the range of the  $e_{ij}$ 's. The approach taken here is to avoid overly disturbing the symmetry by introducing imbalance in the whole terms  $kN_{ij}^1 + e_{ij}$  while maintaining equality of the  $e_i$ 's. Noting from Lemma 2.1 (with  $\rho_2 = 0$ ) that  $\text{var}(\hat{t}_i)$  depends only on  $e_i$  and  $\text{cov}(\hat{t}_i, \hat{t}_j)$  only on  $kN_{ij}^1 + e_{ij}$ , the resulting design will have elementary treatment contrasts estimated with  $m$  distinct variances, where  $m$  is the number of distinct  $kN_{ij}^1 + e_{ij}$ .

Let  $k$  be odd and arbitrarily give the name "end" to one of the vertices of  $K_k$ . Assign the  $k$  treatments of one of the blocks of an initial BIBD  $D_0$  (with parameters as in Theorem 5.1) to the vertices of the graph and decompose it into  $(k - 1)/2$  Hamiltonian cycles. Form two paths of length  $k - 1$ , and hence two ordered blocks, from each cycle by deleting first one of the edges incident with the end vertex, then replacing it and deleting the other. Since the end vertex is adjacent to each other vertex in exactly one cycle,  $e_i = k - 1$  or  $1$  for this set of blocks, where the value is  $k - 1$  if treatment  $i$  is assigned to the end vertex and  $1$  otherwise, and since every other pair of vertices is also adjacent in just one cycle,  $kN_{ij}^1 + e_{ij} = 2k$  or  $2k + 2$  for this set of blocks, where the value is  $2k$  if one of  $i$  and  $j$  corresponds to the end vertex, and  $2k + 2$  otherwise.

Repeating this process for each block of  $D_0$ , all the  $e_i$ 's will be equal if each treatment can be assigned to the end vertex an equal number of times. This is equivalent to choosing one treatment from each block of  $D_0$  as representative of

that block in such a way that each treatment is representative an equal number of times. For this, it is necessary and sufficient that  $b_0 = sv_0$  for some integer  $s \geq 1$  [Hartley, Shrikhande and Taylor (1953)]. The resulting common value for  $e_i$  is  $(k - 1)s + (r_0 - s) = 2s(k - 1)$ .

For  $i \neq j$ , let  $\lambda_{ij}$  be the number of blocks containing both treatments  $i$  and  $j$  for which either  $i$  or  $j$  is the representative. Then in the developed design

$$kN_{ij}^1 + e_{ij} = (2k + 2)(\lambda_0 - \lambda_{ij}) + 2k\lambda_{ij} = 2\lambda_0(k + 1) - 2\lambda_{ij}.$$

A choice of block representatives for a BIBD such that each treatment is a representative an equal number of times and such that the numbers  $\lambda_{ij}$  take on only  $m$  distinct values  $\lambda_1, \lambda_2, \dots, \lambda_m$ , will be called an  $m$ -class representative scheme.

**THEOREM 5.2.** *If there exists a BIBD  $D_0$  with parameters  $b_0 = sv_0$ ,  $v_0$  and  $k_0 = k$  odd, which has an  $m$ -class representative scheme, then there exists a BIBD with parameters  $b = s(k - 1)v$ ,  $v = v_0$  and  $k$  that is partially balanced for the NN1 covariance structure in the sense that elementary treatment contrasts are estimated with  $m$  distinct variances.*

Designs developed according to Theorem 5.2 will be denoted NN1 PBD( $m$ ) or NN1 PBD. With equality of the  $e_i$ 's [ $\text{var}(\hat{t}_i)$ 's], the  $\lambda_{ij}$ 's determine the extent and pattern of dispersion of the elementary contrast variances. In this manner, these designs function in this setting as do the  $m$ -associate class partially balanced incomplete block designs in the setting of uncorrelated errors. However, the representative scheme does not necessarily lead to a PBIBD-type association scheme (although it sometimes does [Morgan (1983)]).

In choosing a representative scheme, the first goal will be to keep the number ( $m$ ) of distinct  $\lambda_{ij}$ 's small; one can then consider other factors such as their range and pattern. In particular, the optimality considerations of the next section demand that the  $\lambda_{ij}$ 's be as equal as possible. We begin with some simple methods for obtaining representative schemes.

**LEMMA 5.1.** *A BIBD with treatment concurrence number  $\lambda$  for which  $v|b$  has a representative scheme with at most  $\min(1 + \lambda, 1 + 2b/v)$  classes.*

**PROOF.** Since  $v|b$ , a set of representatives can be chosen which includes every treatment  $b/v$  times. So a pair of treatments occurs in at most  $2b/v$  blocks for which one is the representative and because the pair occurs in  $\lambda$  blocks, they are in at most  $\lambda$  blocks for which one is the representative.  $\square$

**THEOREM 5.3.** *A BIBD with  $\lambda = 1$  for which  $v|b$  has a two-class representative scheme.*

**THEOREM 5.4.** *A symmetric BIBD has a representative scheme with at most three classes.*

These simple results are quite useful in producing  $NN1$  PBD's with fewer blocks than the corresponding minimum  $NN1$  BIBD's. For instance, if  $t = 2^n$ , the BIBD series with parameters

$$b_0 = v_0 = t^2 + t + 1, \quad k_0 = r_0 = t + 1, \quad \lambda_0 = 1$$

based on  $PG(2, t)$  can be developed to give the  $NN1$  PBD(2) series with

$$\begin{aligned} b &= t(t^2 + t + 1), & v &= t^2 + t + 1, & k &= t + 1, \\ r &= t(t + 1), & \lambda &= t, & \lambda_1 &= 0, & \lambda_2 &= 1 \end{aligned}$$

and a savings of  $t^2 + t + 1$  blocks over the corresponding minimum  $NN1$  BIBDs. Likewise, the symmetric BIBDs with  $v \equiv 3 \pmod{4}$  a prime power and  $k = (v - 1)/2$  may be developed to  $NN1$  PBD's with at most three representative classes and  $v$  fewer blocks than the corresponding minimum  $NN1$  designs.

Another method for finding representative schemes is based on BIBDs cyclically developed from a set of initial blocks. The following is easily proved.

**THEOREM 5.5.** *Suppose that for a BIBD with parameters  $b = sv$ ,  $v$ ,  $k$  and  $\lambda$  cyclically generated from the  $s$  initial blocks  $(a_{i1}, a_{i2}, \dots, a_{ik})$ ,  $i = 1, 2, \dots, s$  (with elements from an additive group), there are elements  $a_{ij}$ ,  $i = 1, 2, \dots, s$  (called initial representatives), such that*

$$\pm(a_{ij} - a_{il}), \quad i = 1, 2, \dots, s, \quad l = 1, 2, \dots, k \text{ and } l \neq j,$$

*are all the nonzero group elements either  $\lambda_1, \lambda_2, \dots$  or  $\lambda_m$  times. Then there is an  $m$ -class representative scheme for the BIBD with parameters  $\lambda_1, \lambda_2, \dots, \lambda_m$ .*

More complicated versions of Theorem 5.5 may be written to cover cases of periodic blocks, fixed elements, etc.

**EXAMPLE 7.**  $B_0 = (0, 6, 8, 9, 11, 15, 25, 32, 33) \pmod{37}$  is a difference set. Since no two elements of  $B_0$  sum to  $0 \pmod{37}$ ,  $0$  may be taken as the initial representative, yielding a two-class scheme with  $\lambda_1 = 0$  and  $\lambda_2 = 1$ .

The choice of any element as initial representative in a difference set necessarily produces a representative scheme with at most three classes; a choice of initial representative yielding two-class schemes has in many cases proved impossible. For  $s = 2$  and  $3$  in Theorem 5.5, trial and error experience has shown that initial representatives yielding three-class schemes are usually easily found.

Now we shall construct some series of designs which will be proved Type II optimal in Section 6. For  $k = v - 1$ , Theorem 5.5 gives a representative scheme with two associate classes. Consider the initial block  $[0, 1, 2, \dots, v - 2]$ . The set of symmetric differences with respect to  $0$  is  $\pm 1, \pm 2, \dots, \pm(v - 2)$  which reduced  $\pmod{v}$  gives the residues  $2, 3, \dots, v - 2$  twice each and the residues  $1$  and  $v - 1$  once each. Hence  $0$  is an appropriate choice for initial representative, giving  $\lambda_1 = 1$  and  $\lambda_2 = 2$ .

As an alternative construction, take  $v/2$  as the initial representative. This choice also yields a two-class representative scheme, but with  $\lambda_1 = 0$  and  $\lambda_2 = 2$ .

**THEOREM 5.6.** *For even  $v$ , there is a symmetric BIBD with  $k = v - 1$  and two-class representative scheme and, hence, an NN1 PBD(2) with parameters*

$$b = v(v - 2), \quad v, \quad k = v - 1, \quad r = (v - 1)(v - 2), \quad \lambda = (v - 2)^2,$$

*which has  $v$  less blocks than the corresponding NN1 minimum optimum design. The parameters of the representative scheme may be taken as  $\lambda_1 = 1, \lambda_2 = 2$  or  $\lambda_1 = 0, \lambda_2 = 2$ .*

Which of the two types of designs is to be recommended? If the experimenter has no interest in the manner of dispersion of variance imbalance across the various pairs of treatments, then the optimality results of Section 6 support the first approach [ $\lambda_1 = 1$ , to be called the "cyclic series," owing to properties of the resultant  $\text{var}(\hat{\mathbf{t}})$ ]. The practical worth to the experimenter of the second construction (to be called the "group divisible series") is found in the pattern it imposes on the off-diagonal elements of  $\text{var}(\hat{\mathbf{t}})$ : The treatments may be divided into  $v/2$  groups of two,  $(i, i + v/2)$  for  $i = 1, 2, \dots, v/2$ , so that comparisons within groups are made with one precision and those between groups with another. If the nature of the treatment set is such that this assignment of the variance imbalance is of value, then this approach should be used.

Now, consider the case  $k = 3$ . If  $v$  is odd, the NN1 minimum optimum designs have parameters  $b = v(v - 1)/2$ ,  $r = 3(v - 1)/2$  and  $\lambda = 3$ . Since  $k - 1 = 2$ , the method of Theorem 5.2 can be used to construct an NN1 PBD with smaller  $b$  only if the initial BIBD satisfies  $v|b$  and  $\lambda = 1$ . Hence one must find representative schemes for BIBD's in the series

$$(5.1) \quad \begin{aligned} b &= v(v - 1)/6, & r &= (v - 1)/2, \\ k &= 3, & \lambda &= 1, & v &\equiv 1 \pmod{6}. \end{aligned}$$

This problem is solved by Theorem 5.3 and the parameters of the representative scheme are  $\lambda_1 = 0$  and  $\lambda_2 = 1$ .

If  $k = 3$  and  $v$  is even, NN1 minimum optimum designs have parameters  $b = v(v - 1)$ ,  $r = 3(v - 1)$  and  $\lambda = 6$ . Theorem 5.2 will produce a design with  $b < v(v - 1)$  for initial BIBD's such that  $v|b$  and  $\lambda = 2$ , that is, for the series

$$(5.2) \quad \begin{aligned} b &= v(v - 1)/3, & r &= (v - 1), & k &= 3, \\ \lambda &= 2, & v &\equiv 4 \pmod{6}. \end{aligned}$$

One construction of this series is given by developing  $(\text{mod } 6t + 3)$  the set of initial blocks  $(0, i, 2t + 1 - i)$ ,  $i = 1, 2, \dots, t$ ,  $(0, 2i, 3t + 1 + i)$ ,  $i = 1, 2, \dots, t$ ,  $(\infty, 0, 3t + 1)$  and  $(0, 2t + 1, 4t + 2)$  of period  $2t + 1$ . It can be verified that the

following choice of representatives yields a two-class representative scheme with  $\lambda_1 = 1$  and  $\lambda_2 = 2$ :

	Block	Representative
(5.3)	$(0, i, 2t + 1 - i)$	$0 =$ initial representative, $i = 1, \dots, t$
	$(0, 2i, 3t + 1 + i)$	$0 =$ initial representative, $i = 1, \dots, t - 1$
	$(0, 2t, 4t + 1)$	$4t + 1 =$ initial representative
	$(\infty, j, 3t + 1 + j)$	$\infty =$ representative, $j = 0, 1, \dots, 2t$
	$(j, 2t + 1 + j, 4t + 2 + j)$	$j =$ representative, $j = 2t + 1, 2t + 2, \dots, 6t + 2$ $j =$ representative, $j = 0, 1, \dots, 2t$

**EXAMPLE 8.**  $t = 1$  in (5.3) gives  $b = 30$ ,  $v = 10$  and  $k = 3$ . The representatives are underlined.

<u>0</u> <u>1</u> <u>2</u> <u>3</u> <u>4</u> <u>5</u> <u>6</u> <u>7</u> <u>8</u>	0 1 2 3 4 5 6 7 8	<u>∞</u> <u>∞</u> <u>∞</u> ∞ ∞ ∞ ∞ ∞ ∞	<u>0</u> <u>1</u> <u>2</u> <u>3</u> <u>4</u> <u>5</u> <u>6</u> <u>7</u> <u>8</u>	<u>0</u> <u>1</u> <u>2</u>
1 2 3 4 5 6 7 8 0	2 3 4 5 6 7 8 0 1	0 1 2 3 4 5 6 7 8	3 4 5	
2 3 4 5 6 7 8 0 1	<u>5</u> <u>6</u> <u>7</u> <u>8</u> <u>0</u> <u>1</u> <u>2</u> <u>3</u> <u>4</u>	4 5 6 7 8 0 1 2 3	6 7 8	

Hamiltonian cycles may also be employed to construct partially balanced  $NN1$  complete block designs. Since variances of estimated contrasts depend only on the  $N_{ij}^1$ , an obvious approach is to keep the  $N_{ij}^1$  “as equal as possible,” and as  $N_{ij}^1 = 1$  ( $i \neq j$ ) is achievable for even  $v$ , only odd  $v$  are considered here. Decompose  $K_v$  into  $(v - 1)/2$  Hamiltonian cycles. Form a path from each cycle by deleting an edge in such a manner that among the vertices that were incident with the set of  $(v - 1)/2$  deleted edges, no one appears more than once (this can always be done). With paths as ordered blocks,  $N_{ij}^1 = 1$  for all but  $(v - 1)/2$  unordered pairs ( $i \neq j$ ) and no treatment is involved in more than one pair such that  $N_{ij}^1 = 0$ . This construction saves just over half of the blocks required for complete balance and it can be shown that the designs enjoy several optimality properties, including Type II optimality and, for  $\rho \geq 0$ ,  $E$ -optimality [Morgan (1983)].

**6. Optimality results for partially variance balanced designs.** The optimality considerations here are essentially the same as in Section 2: Within the class of BIBDs find the optimum designs for least squares estimation under the  $NN1$  model. Because Theorem 2.1 does not apply to the designs of Section 5, Type II optimality is considered and established for the three constructed series of designs  $k = 3$ ,  $k = v - 1$  and  $\lambda_0 = 1$ :

Type II optimality requires minimizing  $\max_{i \neq j} \text{var}(\hat{t}_i - \hat{t}_j)$ . From Lemma 2.1, for a BIBD and the  $NN1$  model, this is equivalent to minimizing  $\max_{i \neq j} \rho[e_i + e_j - (kN_{ij}^1 + e_{ij})]$ . Let  $D_0$  be a BIBD with parameters  $b_0 = sv$ ,  $v_0 = v$ ,  $k_0 = k$ ,  $r_0$  and  $\lambda_0$  and  $m$ -class representative scheme  $(\lambda_1, \lambda_2, \dots, \lambda_m)$ . Development of  $D_0$  according to Theorem 5.2 results in a BIBD with parameters

$$(6.1) \quad b = s(k - 1)v, \quad v, \quad k, \quad r = sk(k - 1) \quad \text{and} \quad \lambda = (k - 1)\lambda_0.$$

For this developed design, the values of  $e_i + e_j - (kN_{ij}^1 + e_{ij})$  are, from Section

5,  $4s(k - 1) - 2\lambda_0(k + 1) + 2\lambda_t$  for  $t = 1, 2, \dots, m$ . If the  $e_i + e_j - (kN_{ij}^1 + e_{ij})$  were all equal, the common value (by averaging over all  $i \neq j$ ) would be

$$4b/v - (2\lambda + 4\lambda/k) = 4s(k - 1) - 2(k + 1)\lambda_0 + 4\lambda_0/k.$$

The differences between this ‘‘optimum’’ value and the attained values are

$$(6.2) \quad 4\lambda_0/k - 2\lambda_t,$$

which will be useful in checking for Type II optimality. More precisely:

**LEMMA 6.1.** *Consider the BIBD with parameters (6.1) obtained by developing a BIBD with  $m$ -class representative scheme  $(\lambda_1, \lambda_2, \dots, \lambda_m)$  according to Theorem 5.2 and suppose  $4\lambda_0 \not\equiv 0 \pmod{k}$ .*

(i) *If  $4\lambda_0/k - 2\lambda_t > -1$ ,  $t = 1, 2, \dots, m$ , the design is Type II optimum for the NN1 model with  $\rho \geq 0$ .*

(ii) *If  $4\lambda_0/k - 2\lambda_t < 1$ ,  $t = 1, 2, \dots, m$ , the design is Type II optimum for the NN1 model with  $\rho \leq 0$ .*

Here we have taken advantage of the fact that  $4\lambda_0/k$  is not integral, while  $e_i + e_j - (kN_{ij}^1 + e_{ij})$  must be: (i) simply means that  $\max_{i \neq j} [e_i + e_j - (kN_{ij}^1 + e_{ij})]$  is as small as possible and (ii) means that  $\min_{i \neq j} [e_i + e_j - (kN_{ij}^1 + e_{ij})]$  is as large as possible. A useful technical lemma (proven in the Appendix) follows.

**LEMMA 6.2.** *A BIBD for which  $v|b$  must have equality of the  $e_i$ 's if either of the following conditions holds:*

$$(6.3) \quad \min_{i \neq j} (e_i + e_j - (kN_{ij}^1 + e_{ij})) \geq \frac{4b}{v} - \text{int} \left( \frac{2b(k - 1)(k + 2)}{v(v - 1)} \right) - 1,$$

$$(6.4) \quad \max_{i \neq j} (e_i + e_j - (kN_{ij}^1 + e_{ij})) \leq \frac{4b}{v} - \text{int} \left( \frac{2b(k - 1)(k + 2)}{v(v - 1)} \right).$$

For designs with parameters (6.1),

$$\text{int}(2b(k - 1)(k + 2)/v(v - 1)) = \text{int}(2\lambda + 4\lambda/k),$$

so for these designs the conditions (6.3) and (6.4) are equivalent to conditions (i) and (ii), respectively, of Lemma 6.1. Now optimality results can be obtained for series of designs from the previous section.

**THEOREM 6.1.** *The series of NN1 PBD(2)'s with parameters  $b = v(v - 1)/3$ ,  $k = 3$ ,  $v = 6t + 1$  ( $t \geq 1$ ),  $\lambda_1 = 0$  and  $\lambda_2 = 1$ , obtained from the BIBD series (5.1), is Type II optimum for the NN1 model.*

**PROOF.** The values of (6.2) are  $4/3$  and  $-2/3$ , so Lemma 6.1 gives the result for  $\rho \geq 0$ . A competitor will perform better for  $\rho < 0$  only if Lemma 6.1(ii) and, hence (6.3), is satisfied so that the  $e_i$ 's must all be equal. Hence the competitor



must satisfy

$$e_{ij} + kN_{ij}^1 \leq \text{int} \left( \frac{2b(k-1)(k+2)}{v(v-1)} \right) + 1 = 7.$$

Since  $k = 3$ ,

$$e_{ij} = 2\lambda - N_{ij}^1 \Rightarrow kN_{ij}^1 + e_{ij} = 4 + 2N_{ij}^1 \leq 7 \Rightarrow N_{ij}^1 \leq 1, \quad i \neq j.$$

But  $\sum_{i \neq j} N_{ij}^1 / v(v-1) = 4/3 \Rightarrow N_{ij}^1 > 1$  for some  $i \neq j$ .  $\square$

**THEOREM 6.2.** *The series of NN1 PBD(2)'s with parameters  $b = 2v(v - 1)/3$ ,  $k = 3$ ,  $v = 6t + 4$  ( $t \geq 0$ ),  $\lambda_1 = 1$  and  $\lambda_2 = 2$ , obtained from the BIBD series (5.2), is Type II optimum for the NN1 model.*

**PROOF.** Similar to the proof of Theorem 6.1.  $\square$

**THEOREM 6.3.** *For  $k = v - 1$  ( $v$  even), the cyclic and group divisible series of NN1 PBD(2)'s are each Type II optimum for the NN1 model with  $\rho \geq 0$ . If  $\rho < 0$ , the cyclic series is superior with respect to the Type II criterion.*

**PROOF.** A direct application of previous results. It should be noted that the cyclic series has less pairs that obtain the Type II bound for  $\rho > 0$  and so may be considered superior in that sense.  $\square$

Calculation of eigenvalues shows that for  $\rho > 0$  the cyclic series is also superior to the group divisible series with respect to  $E$ -optimality (for  $\rho \leq 0$  they are equivalent). With Theorem 6.3, a reasonable argument in favor of the cyclic series is obtained. But as discussed in the previous section, the structure of the group divisible series may be useful for particular sets of treatments, in which case optimality considerations may be secondary.

The final lemma is valuable in showing optimality for those designs with  $\lambda_0 = 1$  (proof in the Appendix).

**LEMMA 6.3.** *A BIBD with parameters  $b = s(k - 1)v$ ,  $v = sk(k - 1) + 1$ ,  $r = sk(k - 1)$ ,  $\lambda = k - 1$  and  $k$  odd, for which all the  $e_i$ 's are equal, satisfies  $kN_{ij}^1 + e_{ij} \leq 2k$  for at least one pair  $i \neq j$ .*

**THEOREM 6.4.** *Developing a BIBD with odd  $k$  and  $\lambda_0 = 1$  by the method of Theorem 5.2 produces a NN1 PBD(2) that is Type II optimum.*

**PROOF.** If  $k = 3$ , the result is given by Theorem 6.1. The values of (6.2) are  $4/k$  and  $4/k - 2$ , so for  $k \geq 5$ , the result for  $\rho \leq 0$  is given by Lemma 6.1.

The values of  $e_i + e_j - (kN_{ij}^1 + e_{ij})$  for this series are  $4b/v - 2k$  and  $4b/v - 2(k + 1)$ . If a competitor is to perform better for  $\rho > 0$ , it must satisfy  $e_i + e_j - (kN_{ij}^1 + e_{ij}) \leq 4b/v - (2k + 1)$  for all  $i \neq j$ , i.e., it must satisfy (6.4). Hence the  $e_i$ 's are all equal and the competitor must satisfy  $e_{ij} + kN_{ij}^1 \geq 2k + 1$  for all  $i \neq j$ , which contradicts Lemma 6.3.  $\square$

APPENDIX

**PROOF OF LEMMA 6.2.** By contradiction. Suppose (6.3) holds and the  $e_i$ 's are not all equal, say  $e_1 = 2b/v - p$ ,  $p > 0$ . Then

$$\begin{aligned}
 kN_{1j}^1 + e_{1j} &\leq e_1 + e_j - \frac{4b}{v} + \text{int}\left(\frac{2b(k-1)(k+2)}{v(v-1)}\right) + 1, \quad j = 2, \dots, v, \\
 \Rightarrow \sum_{j=2}^v (kN_{1j}^1 + e_{1j}) &= 2r(k+1) - \frac{4b}{v} + 2p \leq 2b + (v-2)\left(\frac{2b}{v} - p\right) \\
 &\quad + (v-1)\left[-\frac{4b}{v} + \text{int}\left(\frac{2b(k-1)(k+2)}{v(v-1)}\right) + 1\right].
 \end{aligned}$$

Rearranging gives

$$\begin{aligned}
 p &\leq \frac{(v-1)}{v} \left[ -\frac{2b(k-1)(k+2)}{v(v-1)} + \text{int}\left(\frac{2b(k-1)(k+2)}{v(v-1)}\right) + 1 \right] \\
 &= \frac{(v-1)}{v} \left[ 1 - \text{frac}\left(\frac{2b(k-1)(k+2)}{v(v-1)}\right) \right] < 1.
 \end{aligned}$$

(6.4) is shown similarly.  $\square$

**PROOF OF LEMMA 6.3.** By contradiction. Suppose  $kN_{ij}^1 + e_{ij} \geq 2k + 1$  for all  $i \neq j$ . Since  $\lambda = k - 1$ ,  $0 \leq e_{ij} \leq 2(k - 1)$  and  $0 \leq N_{ij}^1 \leq k - 1$ . Thus  $N_{ij}^1 \geq 1$  for all  $i \neq j$  and

$$N_{ij}^1 = 1 \Rightarrow e_{ij} \geq k + 1.$$

Also, equality of the  $e_i$ 's  $\Rightarrow e_i = 2b/v = 2s(k - 1) \Rightarrow \sum_{j \neq i} N_{ij}^1 = 2r - e_i = 2s(k - 1)^2$ . Let some treatment be given, say treatment 1. Let

$$\begin{aligned}
 a_1 &= \#\{j: N_{1j}^1 = 1, j \in \{2, \dots, v\}\}, \\
 a_2 &= \#\{j: N_{1j}^1 \geq 2, j \in \{2, \dots, v\}\}.
 \end{aligned}$$

Then

$$a_1 + a_2 = v - 1 = sk(k - 1)$$

and

$$\begin{aligned}
 a_1 + 2a_2 &\leq \sum_{j=2}^v N_{1j}^1 = 2s(k - 1)^2 \\
 \Rightarrow a_1 &\geq 2s(k - 1).
 \end{aligned}$$

Hence there are at least  $2s(k - 1)$  treatments  $j$  such that  $e_{1j} \geq k + 1$ .

Let  $A_1$  be the set of blocks containing treatment 1,  $A_1^e$  the subset of  $A_1$  for which 1 is on an end plot and  $A_1^m = A_1 - A_1^e$ . Then

$$\#A_1 = sk(k - 1), \quad \#A_1^e = 2s(k - 1), \quad \#A_1^m = s(k - 1)(k - 2).$$

Let a set  $V_1$  of  $2s(k - 1)$  treatments  $j$  with  $N_{1j}^1 = 1$  be given. These treatments take up  $2s(k - 1)^2$  plots in  $A_1$ . If treatment  $j$  occurs on an end plot of  $A_1^e$ , there

is a contribution of 2 to  $e_{1j}$  and if it occurs on any other plot of  $A_1^e$ , there is a contribution of 1 to  $e_{1j}$ . Occurrence of  $j$  on one of the  $2s(k-1)(k-2)$  end plots of  $A_1^m$  contributes 1 to  $e_{1j}$ ; occurrence on any other plot of  $A_1^m$  makes no contribution. Hence by counting over the  $2s(k-1)^2$  plots,

$$\sum_{j \in V_1} e_{1j} \leq 2[2s(k-1)] + [2s(k-1)^2 - 2s(k-1)] = 2sk(k-1).$$

But since  $N_{1j}^1 = 1 \Rightarrow e_{ij} \geq (k+1)$ , it must hold that

$$\sum_{j \in V_1} e_{1j} \geq 2s(k-1)(k+1),$$

the desired contradiction.  $\square$

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