OPTIMALITY OF SOME TWO-ASSOCIATE-CLASS PARTIALLY BALANCED INCOMPLETE-BLOCK DESIGNS

By C.-S. CHENG¹ AND R. A. BAILEY

University of California, Berkeley, and Rothamsted Experimental Station

Let $\mathscr{D}_{v,\,b,\,k}$ be the set of all the binary equireplicate incomplete-block designs for v treatments in b blocks of size k. It is shown that if $\mathscr{D}_{v,\,b,\,k}$ contains a connected two-associate-class partially balanced design d^* with $\lambda_2=\lambda_1\pm 1$ which has a singular concurrence matrix, then it is optimal over $\mathscr{D}_{v,\,b,\,k}$ with respect to a large class of criteria including the $A,\,D$ and E criteria. The dual of d^* is also optimal over $\mathscr{D}_{b,\,v,\,r}$ with respect to the same criteria, where r=bk/v. The result can be applied to many designs which were not previously known to be optimal. In another application, Bailey's (1988) conjecture on the optimality of Trojan squares over semi-Latin squares is confirmed.

1. Introduction. Let $\mathcal{D}_{v,b,k}$ be the set of all binary equireplicate incomplete-block designs for v treatments in b blocks of size k: each treatment is replicated r times, where r = bk/v. For any $d \in \mathcal{D}_{v,b,k}$, let N_d be the $v \times b$ treatment-block incidence matrix of d. Then the information matrix of d is given by

$$C_d = rI - k^{-1}N_dN_d'.$$

The matrix N_dN_d' is called the concurrence matrix of d and we shall call its off-diagonal entries nontrivial concurrences. It is well known that C_d is symmetric, nonnegative definite and has zero row sums. Optimality criteria are defined as real-valued functions of C_d . Let $\mu_1^d \geq \mu_2^d \geq \cdots \geq \mu_{v-1}^d \geq \mu_v^d = 0$ be the eigenvalues of C_d . Then the commonly used A, D and E criteria seek to minimize $\sum_{i=1}^{v-1} (\mu_i^d)^{-1}$, $\prod_{i=1}^{v-1} (\mu_i^d)^{-1}$ and $(\mu_{v-1}^d)^{-1}$, respectively. It is well known [Kiefer (1975)] that if $\mathcal{D}_{v,b,k}$ contains a balanced incomplete-block design (BIBD) d^* , that is, d^* has all its nontrivial concurrences equal, then d^* is universally optimal over $\mathcal{D}_{v,b,k}$, in the sense defined by Kiefer (1975); in particular, d^* is A, D and E optimal over $\mathcal{D}_{v,b,k}$.

However, for most values of v, b and k there is no BIBD. Two quite separate theories have been developed to deal with this lack. Bose and Nair (1939) and Bose and Shimamoto (1952) introduced partially balanced incomplete-block designs (PBIBD) as a natural extension of BIBD's which had intuitively attractive combinatorial properties and whose algebraic properties enabled efficiency factors to be easily calculated. Most attention has been paid

Received April 1989; revised June 1990.

¹Research supported by NSF Grant DMS-88-02640.

AMS 1980 subject classifications. Primary 62K05; secondary 05B05.

Key words and phrases. Optimal design, partially balanced incomplete-block design, regular graph design, strongly regular graph design.

1667

to PBIBD's with two associate classes, hereafter called PBIB(2) designs. Such a design has precisely two nontrivial concurrences if it is not a BIBD.

Unfortunately, some PBIB(2) designs are not very efficient. An alternative approximation to combinatorial balance is to have precisely two nontrivial concurrences which differ by one. Any such design defines a regular graph whose vertices are the treatments: one concurrence is chosen and there is an edge in the graph between every pair of treatments with the chosen concurrence. John and Mitchell (1977), called such designs regular graph designs (RGD's).

A RGD is a PBIB(2) design if and only if its corresponding graph is strongly regular [Bose (1963)]: we therefore define a strongly regular graph design (SRGD) to be a PBIB(2) design which is also a RGD. It has been conjectured [John and Mitchell (1977); John and Williams (1982)] that if $\mathcal{D}_{v,b,k}$ contains any RGD's, then the optimal RGD's are optimal over the whole of $\mathscr{D}_{n,h,k}$. It is tempting to make a similar conjecture about SRGD's. Indeed, Cheng (1978) has shown that if $\mathscr{D}_{v,b,k}$ contains a group-divisible design d with two groups and $\lambda_2 = \lambda_1 + 1$ (such a design is a SRGD), then d is optimal over $\mathcal{D}_{v,b,k}$ for many criteria, including the A, D and E criteria. However, there is a triangular SRGD which is optimal over all PBIBD(2) designs in $\mathcal{D}_{10,30,2}$ [Cheng (1981a)] but which is inferior to a RGD in $\mathscr{D}_{10,30,2}$ found by John and Mitchell's (1977) computer search.

Although a SRGD is therefore not always optimal over the relevant $\mathcal{D}_{n,h,k}$, we shall show in Theorem 2.2 that many SRGD's are indeed optimal over their $\mathscr{D}_{v,b,k}$ with respect to a large class of criteria. This includes many SRGD's that were not previously known to be optimal: for example, all those with b < vand all the partial geometries introduced by Bose (1963). Section 2 is devoted to the statement, proof and corollary of Theorem 2.2. In Section 3, we apply Theorem 2.2 to a selection of examples. As another application of our results, the conjecture by Bailey (1988) on the optimality of Trojan squares over semi-Latin squares is confirmed.

2. **Results.** Our main theorem is proven by associating each design with a vector \mathbf{x} in *n*-dimensional real space. The coordinates of such a vector are x_1, x_2, \ldots, x_n

THEOREM 2.1. Let \mathscr{C} be a subset of \mathbb{R}^n . Suppose that there is a constant c such that if $\mathbf{x} \in \mathcal{E}$, then $\sum_{i=1}^{n} x_i = c$ and $x_i \geq 0$ for i = 1, ..., n. If \mathcal{E} contains an element **x*** such that:

- (i) $x_i^* > 0$ for i = 1, ..., n;
- (ii) there are two distinct values among x_1^*, \ldots, x_n^* ;
- (iii) \mathbf{x}^* minimizes $\sum_{i=1}^n x_i^2$ over \mathcal{E} ; (iv) \mathbf{x}^* maximizes $\max_{i=1}^n x_i$ over \mathcal{E} ,

then \mathbf{x}^* minimizes $\sum_{i=1}^n f(x_i)$ over \mathscr{C} for all sufficiently differentiable real-valued functions f such that f''(x) > 0, f'''(x) < 0 for x > 0 and $\lim_{x \to 0^+} f(x) =$ $f(0) = \infty$.

The proof of Theorem 2.1 is implicit in Cheng [(1981b), page 246-247] so we do not reproduce it here. We shall consider criteria of the form $\sum_{i=1}^{v-1} f(\mu_i^d)$, where f satisfies the conditions given in Theorem 2.1. The A and D criteria are covered by choosing $f(x) = x^{-1}$ and $-\log x$, respectively, and the E criterion is also covered as a pointwise limit of criteria derived from functions satisfying the conditions in Theorem 2.1.

THEOREM 2.2. If $\mathcal{D}_{v,b,k}$ contains a connected strongly regular graph design d^* whose concurrence matrix is singular, then d^* is optimal over $\mathcal{D}_{v,b,k}$ with respect to any criterion of the form $\sum_{i=1}^{v-1} f(\mu_i^d)$, where f satisfies the conditions given in Theorem 2.1. In particular, d^* is A, D and E optimal over $\mathcal{D}_{v,b,k}$.

PROOF. Let n=v-1. For $d\in \mathscr{D}_{v,b,k}$, put $\mu^d=(\mu_1^d,\ldots,\mu_n^d)$. Let $\mathscr{C}=\{\mu^d:d\in \mathscr{D}_{v,b,k}\}$. For each $d\in \mathscr{D}_{v,b,k}$, we have $C_d=rI\stackrel{.}{-}k^{-1}N_dN_d'$, where r=bk/v. Since d is binary, every diagonal entry of C_d is equal to r(k-1)/k and so $\mu_1^d+\cdots+\mu_n^d=\operatorname{tr}(C_d)=b(k-1)$. Moreover, C_d has no negative eigenvalues. Thus $\mathscr C$ satisfies the conditions of Theorem 2.1.

Write μ_i^* and μ^* for $\mu_i^{d^*}$ and μ^{d^*} . Because d^* is connected, all of μ_1^*,\ldots,μ_n^* are positive. Because d^* is a PBIBD(2), there are two distinct values among μ_1^*,\ldots,μ_n^* [Connor and Clatworthy (1954)]. The trace of C_d^2 is equal to $\sum_{i=1}^n (\mu_i^d)^2$ and this is minimized by any regular graph design [Cheng (1978), page 1246] in $\mathscr{D}_{v,b,k}$, in particular by d^* . We have $r \geq \max_{i=1}^n \mu_i^d = \mu_1^d$. If $N_d N_d'$ is singular, then C_d has at least one eigenvalue equal to r. Hence μ^* maximizes μ_1^d over \mathscr{C} . Therefore, conditions (i)–(iv) of Theorem 2.1 are satisfied.

The result now follows from the conclusion of Theorem 2.1 \Box

COROLLARY 2.3. The dual of the design d^* in Theorem 2.2 is also optimal over $\mathcal{D}_{b,v,r}$ with respect to the same criteria.

PROOF. Denote the dual of d^* by \tilde{d} . Then we have $N_{\tilde{d}}N'_d=N'_{d^*}N_{d^*}$, which has the same nonzero eigenvalues as $N_{d^*}N'_{d^*}$. Since $N_{d^*}N'_{d^*}$ is singular and C_{d^*} has two distinct nonzero eigenvalues, it is clear that $C_{\tilde{d}}$ has at most two distinct nonzero eigenvalues. If $C_{\tilde{d}}$ has only one nonzero eigenvalue, then the optimality of \tilde{d} is obvious. If $C_{\tilde{d}}$ has two distinct nonzero eigenvalues, then $N_{\tilde{d}}N'_{\tilde{d}}$ must be singular. To apply Theorem 2.1 to \tilde{d} , it is sufficient to show that it minimizes tr C_d^2 over $d \in \mathscr{D}_{b,v,r}$. This follows easily from the fact that $\operatorname{tr}(N_dN'_d)^2 = \operatorname{tr}(N'_dN_d)^2$ and that d^* minimizes tr C_d^2 over $d \in \mathscr{D}_{v,b,k}$. \square

3. Applications. The results in Section 2 cover many PBIB(2) designs which were not proven optimal before. In the following, we shall give a list of some PBIB(2) designs to which Theorem 2.2 can be applied.

Theorem 2.2 and Corollary 2.3 establish the optimality of PBIB(2) designs with $\lambda_2 = \lambda_1 \pm 1$ which have singular concurrence matrices, and their duals. These include, for example, the following designs and their duals: (i) all the PBIB(2) designs with $\lambda_2 = \lambda_1 \pm 1$ and b < v; (ii) all the resolvable PBIB(2)

designs with $\lambda_2 = \lambda_1 \pm 1$ and b < v + r - 1; (iii) all the partial geometries introduced by Bose (1963); (iv) all the singular group-divisible designs with $\lambda_2 = \lambda_1 - 1$; (v) all the semiregular group-divisible designs with $\lambda_2 = \lambda_1 + 1$. The readers are referred to Raghavarao (1971) or Clatworthy (1973) for the definitions of these designs. Comprehensive tables of PBIB(2) designs can be found in Clatworthy (1973).

Some families of semiregular group-divisible designs with $\lambda_2 = \lambda_1 + 1$ have been reported in the literature. For example, Bose, Shrikhande and Bhattacharya (1953) constructed, for every prime or prime power s and any m < s + 1, a semiregular group-divisible design with v = ms, $b = s^2$, k = m, $\lambda_1 = 0$ and $\lambda_2 = 1$. Raghavarao [(1971), page 140] reported a family of semiregular group-divisible designs with $v = s^3$, $b = s^2(s + 1)$, $k = s^2$, $\lambda_1 = s$ and $\lambda_2 = s + 1$ for any prime or prime power s, which can be constructed by a method described in Bose, Shrikhande and Bhattacharya (1953).

The lattice designs introduced by Yates (1936) are popular in practice because they are resolvable and easy to construct. For $b \le v$, they are L_r -type PBIB(2) designs with $\lambda_1 = 1$ and $\lambda_2 = 0$, where r is the replication and their concurrence matrices are singular. Patterson and Williams (1976) proved that these designs are A-optimal among resolvable designs. Theorem 2.2 improves this result in two ways: it extends the class of optimality criteria and removes the restriction to resolvability for the competing designs.

Triangular type PBIB(2) designs with $\lambda_2 = \lambda_1 \pm 1$ which have singular concurrence matrices can also be found. One such example is design T16 in Clatworthy (1973) with parameters v = b = 15, k = 3, $\lambda_1 = 0$, $\lambda_2 = 1$.

Many of the triangular and L_2 -type PBIB(2) designs with $\lambda_2 = \lambda_1 \pm 1$ which have singular concurrence matrices have b < v or are duals of BIBDs or semiregular group-divisible designs with $\lambda_2 = \lambda_1 + 1$. So their optimality can also be obtained by other means. Design T16 has v = b and is truly self dual, that is, it is isomorphic to its dual; therefore its optimality does not follow from that of a previously known optimal design.

It is interesting to observe that if a design satisfies the conditions of Theorem 2.2, then its complement also satisfies these conditions. So we have the situation where a design and its complement are both optimal, which is not true in general.

Another application of our results is to show the optimality of Trojan squares over semi-Latin squares. Bailey (1988) discussed the use of semi-Latin squares in the experimental situation where k plots are nested in each cell of an $n \times n$ square. Suppose there are nk treatments. Then in a semi-Latin square, the nk treatments are allocated to plots in such a way that each row and each column is a complete replicate of the treatments. For convenience, the k observations nested in each row-column intersection are called a block. A Trojan square is a special kind of semi-Latin square defined by taking k mutually orthogonal $n \times n$ Latin squares on k disjoint sets of treatments; each block of the semi-Latin square contains the treatments which occur in the corresponding cell of all the individual Latin squares. Because of the orthogonality between treatments, rows and columns, the information matrix (in the plots stratum) of a semi-Latin square is identical to the C-matrix of the

block design consisting of the n^2 blocks of size k; see Bailey (1988) for details. Bailey (1988) conjectured that a Trojan square is optimal (for analysis in the plots stratum) over semi-Latin squares. It is easy to see that the n^2 blocks of a Trojan square are a semiregular group-divisible design with $\lambda_1 = 0$ and $\lambda_2 = 1$. Therefore it is optimal with respect to the criteria described in Theorem 2.2; in particular it is A, D, and E optimal.

Acknowledgments. The authors are grateful to the Institute for Mathematics and Its Applications, University of Minnesota, where this work was begun, for its hospitality, and to J. van Lint and A. Blokhuis for helpful discussions on strongly regular graphs.

REFERENCES

- Bailey, R. A. (1988). Semi-Latin squares. J. Statist. Plann. Inference 18 299-312.
- Bose, R. C. (1963). Strongly regular graphs, partial geometries and partially balanced designs. Pacific J. Math. 13 389-419.
- Bose, R. C. and Nair, K. R. (1939). Partially balanced incomplete block designs. Sankhyā 4 337-372.
- Bose, R. C. and Shimamoto, T. (1952). Classification and analysis of partially balanced incomplete block designs with two associate classes. J. Amer. Statist. Assoc. 47 151–184.
- Bose, R. C., Shrikhande, S. S. and Bhattacharya, K. N. (1953). On the construction of group divisible incomplete block designs. *Ann. Math. Statist.* **24** 167–195.
- CHENG, C.-S. (1978). Optimality of certain asymmetrical experimental designs. Ann. Statist. 6 1239-1261.
- CHENG, C.-S. (1981a). On the comparison of PBIB designs with two associate classes. *Ann. Inst. Statist. Math.* **33** 155-164.
- CHENG, C.-S. (1981b). Maximizing the total number of spanning trees in a graph: two related problems in graph theory and optimum design theory. J. Combin. Theory Ser. B 31 240-248.
- CLATWORTHY, W. H. (1973). Tables of two-associate-class partially balanced designs. NBS Applied Mathematics Series 63, National Bureau of Standards, Washington, DC.
- CONNOR, W. S. and CLATWORTHY, W. H. (1954). Some theorems for partially balanced designs.

 Ann. Math. Statist. 25 100-112.
- JOHN, J. A. and MITCHELL, T. J. (1977). Optimal incomplete block designs. J. Roy. Statist. Soc. Ser. B 39 39-43.
- JOHN, J. A. and WILLIAMS, E. R. (1982). Conjectures for optimal block designs. J. Roy. Statist. Soc. Ser. B 44 221-225.
- KIEFER, J. (1975). Construction and optimality of generalized Youden designs. In A Survey of Statistical Designs and Linear Models (J. N. Srivastava, ed.) 333-353. North-Holland, Amsterdam.
- Patterson, H. D. and Williams, E. R. (1976). Some theoretical results on general block designs. In *Proceedings of the Fifth British Combinatorial Conference* (C. St. J. A. Nash-Williams and J. Sheehan, eds.) 489-496. Utilitas Mathematica, Winnepeg.
- RAGHAVARAO, D. (1971). Constructions and Combinatorial Problems in Design of Experiments. Wiley, New York.
- YATES, F. (1936). A new method of arranging variety trials involving a large number of varieties.

 Journal of Agricultural Science 26 424-455.

DEPARTMENT OF STATISTICS UNIVERSITY OF CALIFORNIA BERKELEY, CALIFORNIA 94720 DEPARTMENT OF MATHEMATICAL SCIENCES GOLDSMITH'S COLLEGE NEW CROSS LONDON SE14 6NW ENGLAND