OPTIMAL BLOCK DESIGNS FOR TRIALLEL CROSS EXPERIMENTS

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Key Words: Nested designs; Balanced block designs; Optimality

ABSTRACT

Optimal block designs for a certain type of triallel cross experiments are investigated. Nested balanced block designs are introduced and it is shown how these designs give rise to optimal designs for triallel crosses. Several series of nested balanced block designs, leading to optimal designs for triallel crosses are reported.

1 INTRODUCTION

Triallel crosses are a type of mating design used to study the genetic properties of a set of inbred (pure) lines in plant breeding. Suppose there are p inbred lines and it is desired to perform a triallel cross involving some or all of $n_c = p(p-1)(p-2)/3$ possible crosses of the type $(i \times j \times l)$, $i < j < l$, $i, j, l = 1, 2, \ldots, p$. Let n denote the total number of crosses (experimental units) involved in a triallel cross experiment. It is desired to compare the lines with respect to their general combining abilities, the specific combining abilities being not included in the model. Triallel crosses are discussed by Hinkelmann (1965), Arora and Aggarwal (1984, 1989), Ceranka et. al (1990) and Ponnuswamy and Srinivasan (1991). Customarily, triallel crosses have been conducted using a completely randomised design or a randomised complete block design involving n_c treatments. However, with increase in the number of lines p, the number of crosses, n_c, in the experiment increases rapidly. Thus, if p is large adoption of an unblocked design or a complete block design is not appropriate unless the experimental units are extremely homogeneous. Following the approach of Gupta and Kageyama (1994), and Dey and Midha (1996), we start with p, the number of lines, rather than n_c, the total number of distinct crosses in the experiment. This approach yields optimal designs involving n experimental units where $n < n_c$.

The purpose of this communication is to investigate the problem of obtaining optimal designs for triallel crosses. The optimality criterion chosen is the universal optimality criterion of Kiefer (1975) which, in particular, includes the minimization of the average variance of the best linear unbiased estimators of all elementary comparisons between the general combining ability effects of the lines involved. In Section 2, a class of designs, called the class of nested balanced block designs is shown to be useful for the construction of optimal designs for triallel crosses in incomplete blocks. In Section 3, several families of such designs are reported.

2 OPTIMALITY TOOLS

Let d be a block design for a triallel cross experiment involving p inbred lines, b blocks each of size k. This means that there are k crosses in each of the blocks of d. Further, let r_{di} denote the number of times the ith cross appears in d, $i = 1, 2, \ldots, p(p-1)(p-2)/3$, and similarly, let s_{dj} denote the number of times the jth line occurs in crosses in the whole design d, $j = 1, 2, \ldots, p$. Then, $\sum r_{di} = bk$ and $\sum s_{dj} = 3bk$. Also, $n = bk$ is the number of observations generated by d. For the data obtained from the design d, we postulate the model

$$Y = \mu 1_n + \Delta_1 \boldsymbol{g} + \Delta_2 \boldsymbol{\beta} + \boldsymbol{\epsilon}, \tag{2.1}$$

where $\mathbf{Y}$ is the $n \times 1$ vector of observed responses, μ is a general mean effect, 1_n denotes an $n-$component column vector of all ones, $\boldsymbol{g}$ and $\boldsymbol{\beta}$ are vectors of p general combining ability effects and b block effects respectively, Δ_1, Δ_2 are the corresponding design matrices, that is, the (α, β)th element of Δ_1 (respectively, of Δ_2) is 1 if the αth observation pertains to the βth line (respectively, to the βth block), and is zero otherwise; $\boldsymbol{\epsilon}$ is the vector of random error components, these components being distributed with mean zero and constant variance σ^2. In (2.1), we have not included the specific combining ability effects. Under the model (2.1), it can be shown that the coefficient matrix of the reduced normal equations for estimating linear functions of general combining ability effects, using a design d, is

$$C_d = G_d - N_d N_d'/k \tag{2.2}$$

where $G_d = (g_{dii'})$, $N_d = (n_{dij})$, $g_{dii} = s_{di}$, and for $i \neq i'$, $g_{dii'}$ is the number of crosses in d in which i and i' appear together; n_{dij} is the number of times the line i occurs in block j of d.

A design d will be called *connected* if and only if $Rank(C_d) = p - 1$, or equivalently, if and only if all elementary comparisons among general combining ability effects are estimable using d. We denote by $\mathcal{D}(p, b, k)$ the class of all such connected block designs $\{d\}$ with p lines, b blocks each of size k. We need the following well known lemma.

Lemma 2.1 For given positive integers s and t, the minimum of $\sum_{i=1}^{s} n_i^2$

subject to $\sum_{i=1}^{s} n_i = t$, where n_i's are non-negative integers, is obtained when $t - s[t/s]$ of the n_i's are equal to $[t/s]+1$ and $s - t + s[t/s]$ are equal to $[t/s]$, where $[z]$ denotes the largest integer not exceeding z. The corresponding minimum of $\sum_{i=1}^{s} n_i^2$ is $t(2[t/s]+1) - s[t/s]([t/s]+1)$.

We then have

Theorem 2.1 For any design $d \in \mathcal{D}(p,b,k)$,

$$tr(C_d) \;\leq\; k^{-1}b\{3k(k-1-2x)+px(x+1)\},$$

where $x = [3k/p]$ and for a square matrix A, $tr(A)$ stands for the trace.

Proof. For any $d \in \mathcal{D}(p,b,k)$, we have

$$\begin{aligned} tr(C_d) &= \sum_{i=1}^{p} s_{di} - k^{-1}\sum_{i=1}^{p}\sum_{j=1}^{b} n_{dij}^2 \\ &= 3bk - k^{-1}\sum_{i=1}^{p}\sum_{j=1}^{b} n_{dij}^2. \end{aligned}$$

Now, since $\sum_{i=1}^{p}\sum_{j=1}^{b} n_{dij} = 3bk$, using Lemma 2.1,

$$\sum_{i=1}^{p}\sum_{j=1}^{b} n_{dij}^2 \;\geq\; b\{3k(2x+1)-px(x+1)\}, \;\; where \;\; x = [3k/p].$$

Hence,

$$\begin{aligned} tr(C_d) &\leq 3bk - k^{-1}b\{3k(2x+1)-px(x+1)\} \\ &= k^{-1}b\{3k(k-1-2x)+px(x+1)\}. \end{aligned}$$

By Lemma 2.1, equality above is attained if and only if $n_{dij} = x \;\; or \;\; x+1$, for $i = 1,2,\ldots,p; j = 1,2,\ldots,b$.

Corollary 2.1 For any design $d \in \mathcal{D}(p,b,k)$, $\;if\;\; 3k/p \geq 1$ (i.e., $x \geq 1$) then

$$tr(C_d) \leq k^{-1}b\{3k(k-1-2x)+px(x+1)\} \leq 3bk(p-3)/p \leq 3b(k-1).$$

Also, if $3k/p < 1$ (i.e., $x = 0$) then $tr(C_d) \leq 3b(k-1)$.

Corollary 2.2 Let $B_1 = k^{-1}b\{3k(k-1-2x)+px(x+1)\}$, $B_2 = 3bk(p-3)/p$ and $B_3 = 3b(k-1)$. Then for any $d \in \mathcal{D}(p,b,k)$ with $3k \geq p$, $tr(C_d) \leq B_1 \leq B_2 \leq B_3$ and the following hold:
(a) $tr(C_d)$ attains the value B_1 if $n_{dij} = x \ \ or \ \ x+1, \ \ \forall \ \ i,j$.
(b) $tr(C_d)$ attains the value B_2 if $n_{dij} = 3k/p \ \ \forall \ \ i,j$. In such a situation, $B_1 = B_2$ and $x = [3k/p] = 3k/p$.
(c) $tr(C_d)$ attains the value B_3 if $n_{dij} = 0 \ \ or \ \ 1 \ \ \forall \ \ i,j$. If $n_{dij} = 1$ for all i,j, then $B_1 = B_2 = B_3$ and $x = 3k/p = 1$.

Kiefer (1975) showed that a design is universally optimal in a relevant class of competing designs if (i) the information matrix (the C-matrix) of the design is completely symmetric in the sense that C has all its diagonal elements equal and all its off-diagonal elements equal, and (ii) the matrix C has maximum trace over all designs in the class of competing designs. Recall that a universally optimal design is in particular, also A−optimal, that is, such a design minimizes the average variance of the best linear unbiased estimators of all elementary contrasts among the parameters of interest (the general combining ability effects, in our context). Making an appeal to this result of Kiefer (1975) and to Theorem 2.1, we have the following result.

Theorem 2.2 Let $d^* \in \mathcal{D}(p,b,k)$ be a block design for triallel crosses, satisfying
(i) $tr(C_{d^*}) = k^{-1}b\{3k(k-1-2x)+px(x+1)\}$, and (ii) C_{d^*} is completely symmetric. Then d^* is universally optimal in $\mathcal{D}(p,b,k)$, and in particular minimizes the average variance of the best linear unbiased estimators of all elementary contrasts among the general combining ability effects.

We recall the definition of a balanced block design (cf. Kiefer (1958), Das and Dey (1989)).

Definition 2.1 Let d be a block design with $v \geq 3$ treatments and b blocks, each of size $k \geq 2$ and suppose $N_d = (n_{dij})$ is the incidence matrix of d. Then d is called a balanced block design if (i) $\sum_{j=1}^{b} n_{dij} n_{dmj} = \lambda$, for $i \neq m$, $i, m = 1, 2, \ldots, v$ and (ii) $|n_{dij} - k/v| < 1$, $\forall\ i, j$.

For a balanced block design each treatment is replicated $r = bk/v$ times and the parameters of the design are v, b, r, k, λ. A balanced block design with $k < v$ is a balanced incomplete block (BIB) design. Based on the above, we now have the following definition which is a generalization of nested BIB designs of Preece(1967).

Definition 2.2 Let d be a balanced block design with v treatments and b_1 blocks each of size $k_1 \geq 4$. Further, let it be possible to partition each block of d into sub-blocks, each of size $k_2 \geq 2$. If these sub-blocks, say b_2 in number, also form a balanced block design, then d will be called a nested balanced block design with parameters v, b_1, b_2, k_1, k_2.

A nested balanced block design design with $k_1 < v$ is a nested BIB design.

Consider now a nested balanced block design d_1 with parameters $v = p, b_1, b_2, k_1, k_2 = 3$. If we now identify the treatments of d_1 as lines of a triallel experiment and perform crosses among the lines appearing in the same sub-block of d_1, we get a block design d^* for a triallel experiment involving p lines with $n = b_2$ crosses, arranged in $b = b_1$ blocks, each of size $k = k_1/3$. Such a design $d^* \in \mathcal{D}(p, b, k)$ and

$$C_{d^*} = (p-1)^{-1} k^{-1} b\{3k(k-1-2x) + px(x+1)\}(I_p - p^{-1} J_p), \qquad (2.3)$$

where $x = [3k/p]$, I_p is an identity matrix of order p and J_p is a $p \times p$ matrix of all ones. Furthermore, using d^*, all elementary contrasts among general combining ability effects are estimated with a variance $2b^{-1}(p-1)k\sigma^2/\{3k(k-1-2x) + px(x+1)\}$.

From (2.3) and Theorem 2.2, we thus get the following result.

Theorem 2.3 Let $d^* \in \mathcal{D}(p, b, k)$ be a design constructed using a nested balanced block design with parameters $v = p, b_1 = b, b_2 = bk, k_1 = 3k, k_2 =$

3. Then d^* is universally optimal in $\mathcal{D}(p, b, k)$ and thus minimizes the average variance of the best linear unbiased estimators of all elementary contrasts among the general combining ability effects.

3 CLASSES OF OPTIMAL DESIGNS

In this section, we present several classes of universally optimal mating designs for triallel crosses. Throughout this section, we consider nested balanced block designs with sub-blocks of size three each, i.e., $k_2 = 3$, and hence present the parameters of the nested balanced block design in terms of p, b, k_1, where p denotes the number of treatments, b denotes the number of blocks in the design, and k_1 is the size of the block. Families 2–4 make use of the nested BIB designs given by Dey, et. al (1986).

Family 1. Let $p = 6t + 3$, where $t \geq 1$ is an integer. There exists an optimal mating design with parameters $p = 6t+3, n = (2t+1)(3t+1), b = 3t+1, k = 2t+1$.

A particular class of BIB designs is the Resolvable Steiner's triple systems with parameters $v = 6t+3, b_2 = (3t+1)(2t+1), r = 3t+1, k_2 = 3, \lambda = 1$ have been given by Raychaudhuri and Wilson (1968). Taking each replication as one block with $2t + 1$ sub-blocks of this Steiner's triple system which form the replicate, we get a nested balanced block design leading to an optimal mating design of the above family.

Example 3.1 Let $t = 1$. Then a resolvable Steiner's triple system with parameters $v = 9, b = 12, r = 4, k = 3, \lambda = 1$ provides a Family 1 mating design as shown below:

$$\{(1,2,3),\ (4,5,6),\ (7,8,9)\};$$
$$\{(1,4,7),\ (2,5,8),\ (3,6,9)\};$$
$$\{(1,6,8),\ (2,4,9),\ (3,5,7)\};$$
$$\{(1,5,9),\ (2,6,7),\ (3,4,8)\};$$

The design has 12 crosses in 4 blocks each of size 3, by making crosses between the lines within each sub-block. For instance, the first block of the design for triallel crosses will have the following crosses:

$$[1 \times 2 \times 3, \quad 4 \times 5 \times 6, \quad 7 \times 8 \times 9].$$

Family 2. The existence of a BIB design D_1 with parameters $p, b, r, k_1 = 6t+3, \lambda$, where $t \geq 1$ is an integer, implies the existence of an optimal mating design with parameters $p, n = b(2t+1)(3t+1), b = b(3t+1), k = 2t+1$.

Construct a Family 1 mating design using the symbols in the ith block of $D_1, i = 1, 2, \ldots, b$. A Family 2 design is obtained by taking together all the blocks obtained in this manner.

Family 3. The existence of a BIB design D_1 with parameters $v = 2t+1, b_1, r_1, k_1, \lambda$, where $t \geq 1$ is an integer, implies the existence of an optimal mating design with parameters $p = 6t+3, n = b_1 k_1(3t+1), b = b_1(3t+1), k = k_1$.

Let D_2 be a Family 1 mating design. Construct a mating design by replacing the ith treatment of D_1 by the ith block contents of the first block of $D_2, i = 1, 2, \ldots, 2t+1$. Do this for each of the $3t+1$ blocks of D_2. The resulting design belongs to Family 3.

Example 3.2 Take D_2 as the mating design given in Example 3.1, and let D_1 be the BIB design (1,2), (1,3), (2,3). Then a Family 3 mating design is as shown below:

$$\{(1,2,3),(4,5,6)\}; \quad \{(1,2,3),(7,8,9)\}; \quad \{(4,5,6),(7,8,9)\};$$
$$\{(1,4,7),(2,5,8)\}; \quad \{(1,4,7),(3,6,9)\}; \quad \{(2,5,8),(3,6,9)\};$$
$$\{(1,6,8),(2,4,9)\}; \quad \{(1,6,8),(3,5,7)\}; \quad \{(2,4,9),(3,5,7)\};$$
$$\{(1,5,9),(2,6,7)\}; \quad \{(1,5,9),(3,4,8)\}; \quad \{(2,6,7),(3,4,8)\}.$$

The design has 24 crosses in 12 blocks of size two.

In addition to the resolvable Steiner's triple systems, there may exist other resolvable BIB designs with block size three, e.g., the BIB design with parameters $v = 6, b = 20, r = 10, k = 3, \lambda = 4$. Some further optimal mating designs can be obtained by using such resolvable BIB designs in place of the Steiner's triple systems in the above three families.

Family 4. Let $p = 6t + 1$ be a prime or a prime power and let x be a primitive element of GF(p). Then by developing the initial block mod(p):

$$\{(x^i, x^{i+2t}, x^{i+4t}), (x^{i+t}, x^{i+3t}, x^{i+5t})\} \qquad i = 0, 1, \ldots, t-1,$$

we get an optimal mating design with parameters $p = 6t + 1, n = 2p, b = p, k = 2t$, the lines being coded as 0,1,2,. . . , p -1.

Example 3.3 Let $t = 1$. Then $x = 3$ is a primitive element of $p = 7$. The following optimal design involving 14 crosses in blocks of size 2 belongs to Family 4:

$$\{(1,2,4), \ (3,6,5)\};$$
$$\{(2,3,5), \ (4,0,6)\};$$
$$\{(3,4,6), \ (5,1,0)\};$$
$$\{(4,5,0), \ (6,2,1)\};$$
$$\{(5,6,1), \ (0,3,2)\};$$
$$\{(6,0,2), \ (1,4,3)\};$$
$$\{(0,1,3), \ (2,5,4)\};$$

Some optimal mating designs can be obtained using α-resolvable BIB designs. For instance, if each block of a BIB design is repeated s times than trivially we can get a α-resolvable BIB design with $\alpha = r$. Below we give an example of $s = 2$. Such designs can be trivially constructed but they may be useful in some practical situations.

Example 3.4 By taking $s = 2$ replications of the BIB design with parameters $v = b = 7, r = k_1 = 3, \lambda = 1$ we can get a 3-resolvable BIB design with parameters $v = 7, b = 14, r = 6, k_1 = 3, \lambda = 2$. Then we can construct the following optimal mating design for $p = 7$, consisting of 14 crosses in two blocks of size 7 each:

$$\{(1,2,4),\ (2,3,5),\ (3,4,6),\ (4,5,7),\ (5,6,1),\ (6,7,2),\ (7,1,3)\};$$
$$\{(1,2,4),\ (2,3,5),\ (3,4,6),\ (4,5,7),\ (5,6,1),\ (6,7,2),\ (7,1,3)\}.$$

Some optimal mating designs can be obtained using nested balanced incomplete block designs with sub-blocks of size 3 each listed by Preece (1967). We provide these mating designs in the following table where the Reference column gives the serial numbers of designs from Table 3 of Preece (1967).

Table

Parameters of some optimal mating designs

p	n	b	k	Reference
10	30	10	3	5(i)
19	57	19	3	6
12	44	22	2	9(i)
13	52	26	2	10(ii)
13	52	13	4	10(i)
27	117	39	3	11
15	70	35	2	12
16	80	16	5	13
31	93	31	3	14

ACKNOWLEDGEMENTS

The authors are thankful to Professors Aloke Dey, Sanpei Kageyama and Rahul Mukerjee for some helpful discussions.

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