Chapter 2

Preliminaries

The diallel cross experiments involving $p(p+1)/2$ distinct crosses are considered. Let d be a block design for a diallel cross experiment with p test lines, one control line, and b blocks of size k each. Let s_{di} denote the number of times line i occurs in crosses in d, i = 0, 1, … , p, let $g_{dii'}$ denote the number of times the cross (i, i') appears in d, $\forall\ i \neq i'$, i, i' = 0, 1, … , p, and let n = bk denote the total number of crosses in d. The model for design d is then assumed to be

$$\vec{Y}_d = \mu\vec{1}_n + \Delta_{1d}\vec{\tau} + \Delta_{2d}\vec{\beta} + \vec{\varepsilon} \,,$$

where $\vec{Y}_d$ is the $n \times 1$ vector of observed responses, μ is the overall mean, $\vec{1}_n$ denotes the $n \times 1$ vector of 1's, $\vec{\tau} = (\tau_0, \tau_1, \cdots, \tau_p)'$ is the vector of p + 1 general combining ability effects, $\vec{\beta} = (\beta_1, \cdots, \beta_b)'$ is the vector of b block effects, Δ_{1d}, Δ_{2d} are the corresponding design matrices, that is, the (s,h)th elememt of Δ_{1d} is 1 if the sth observation pertains to line h, and is zero, otherwise; and the (s,l)th element of Δ_{2d} is 1 if the sth observation pertains to block l, and is zero, otherwise; $\vec{\varepsilon}$ is the $n \times 1$ vector of uncorrelated random errors with mean zero and constant variance σ^2. The coefficient matrix of the reduced normal equations for estimating $\vec{\tau}$ is

$$C_d = G_d - (1/k)N_d N_d' \,,$$

where $G_d = \Delta'_{1d}\Delta_{1d} = (g_{dii'})$, $g_{dii} = s_{di}$, and $N_d = \Delta'_{1d}\Delta_{2d} = (n_{dij})$, n_{dij} is the number of times line *i* occurs in block *j*. Note that the row sums and column sums of C_d are all zero. In this thesis, our focus is on the estimation of the test line versus control contrasts $(\tau_1 - \tau_0, \cdots, \tau_p - \tau_0)'$, and by Bechhofer and Tamhane (1981), and Das, Gupta, and Kageyama (2002), the information matrix, $M_d = (m_{dii'})$, for the estimation of $(\tau_1 - \tau_0, \cdots, \tau_p - \tau_0)'$ is obtained by deleting the first row and first column of C_d, and

$$M_d = \begin{cases} s_{di} - (1/k)\sum_{j=1}^{b} n_{dij}^2 & \text{, for } i = i' \\ g_{dii'} - (1/k)\sum_{j=1}^{b} n_{dij}n_{di'j} & \text{, for } i \neq i' \end{cases}.$$

Let $D(p+1,b,k)$ be a collection of all connected designs with *p* test lines, one control line, *b* blocks of size *k*. A design $d^* \in D(p+1,b,k)$ is said to be A-optimal if it minimizes $\sum_{i=1}^{p} Var(\hat{\tau}_i - \hat{\tau}_0)$, where $\hat{\tau}_i - \hat{\tau}_0$ is the best linear unbiased estimator (BLUE) of $\tau_i - \tau_0$, i = 1, … , *p*, over all designs in $D(p+1,b,k)$, that is, *d** satisfies

$$\sum_{i=1}^{p} Var(\hat{\tau}_{d^*i} - \hat{\tau}_{d^*0}) = \min_{d \in D(p+1,b,k)} \sum_{i=1}^{p} Var(\hat{\tau}_{di} - \hat{\tau}_{d0}), \text{ or}$$

$$trM_{d^*}^{-1} = \min_{d \in D(p+1,b,k)} trM_d^{-1}.$$

For a design $d \in D(p+1,b,k)$, applying the averaging technique in Kiefer (1975), Majumdar and Notz (1983), and Jacroux and Majumdar (1989), one can show that

$$trM_d^{-1} \geq tr\overline{M}_d^{-1},$$

where $\overline{M}_d = (1/p!)\sum_{\pi} \pi \overline{M}_d \pi'$, is the average of all possible permutations of the

p test lines on M_d, and π is the corresponding $p \times p$ permutation matrix. We should note that $\overline{M}_d$ is completely symmetric, that is, $\overline{M}_d = aI_p + bJ_{p,p}$, where I_p is the $p \times p$ identity matrix, and $J_{p,p}$ is a $p \times p$ matrix of 1's. Among all designs in $D(p+1,b,k)$, a group of designs having completely symmetric information matrices is called a type S block design by Choi, Gupta, and Kageyama (2002).

Definition 2.1. (Choi, Gupta, and Kageyama (2002)) A design $d \in D(p+1,b,k)$ is a type S block design if $\forall\, i \neq i' = 1, \ldots, p$, $g_{d0i} = g_0$, $g_{dii'} = g_1$, $\sum_{j=1}^{b} n_{d0j} n_{dij} = \lambda_0$, and $\sum_{j=1}^{b} n_{dij} n_{di'j} = \lambda_1$, where g_0, g_1, λ_0, and λ_1 are integers.

A type S block design if it further satisfies that the control line as well as the p test lines appears as evenly as possible in each block is called a type S_0 block design by Das, Gupta, and Kageyama (2002), and their A-optimality property has also been shown.

Definition 2.2. (Das, Gupta, and Kageyama (2002)) A type S block design d is said to be a type S_0 block design, denoted as $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$, if it satisfies $|n_{d0j} - n_{d0j'}| \leq 1$, $|n_{dij} - n_{di'j'}| \leq 1$, for $i, i' = 1, \ldots, p$; $j, j' = 1, \ldots, b$.

Through straightforward calculation, a type S_0 block design d has the following properties.

(i) $s_{d0} = pg_0$,

(ii) $s_{d1} = \cdots = s_{dp} = g_0 + (p-1)g_1 = s_1$, say,

(iii) $pg_0 + (p(p-1)/2)g_1 = bk$,

(iv) $\sum_{j=1}^{b} n_{d0j}^2 = p(2kg_0 - \lambda_0)$,

(v) $\sum_{j=1}^{b} n_{dij}^2 = 2k\big(g_0 + (p-1)g_1\big) - (p-1)\lambda_1 - \lambda_0$, $i = 1, \ldots, p$,

(vi) $M_d = \big((p\lambda_1 + \lambda_0)/k - g_0 - pg_1\big)I_p + (g_1 - \lambda_1/k)J_p$, and

the eigenvalues μ_{di} , $i = 1, \ldots, p$, of M_d are $\mu_{d1} = \lambda_0/k - g_0$,

$\mu_{d2} = \cdots = \mu_{dp} = (\lambda_0 + p\lambda_1)/k - g_0 - pg_1$.

Let

$$g(s_{d0}; p, b, k) = \frac{p}{s_{d0} - h(s_{d0})/k} + \frac{(p-1)^2}{2bk - s_{d0} - a(s_{d0})/k - (s_{d0} - h(s_{d0})/k)/p},$$

where $a(s_{d0}) = (2bk - s_{d0})(2y_1 + 1) - pby_1(y_1 + 1)$, $h(s_{d0}) = s_{d0}(2y_2 + 1) - by_2(y_2 + 1)$, $y_1 = [(2bk - s_{d0})/pb]$, $y_2 = [s_{d0}/b]$, and $[\cdot]$ is the greatest integer function. Das, Gupta, and Kageyama (2002) show that for a design $d \in D(p+1, b, k)$, $trM_d^{-1} \geq tr\overline{M}_d^{-1} \geq g(s_{d0}; p, b, k)$, and the equalities holds when M_d is completely symmetric. Using the above inequality, the A-optimality of type S_0 block design is thus proved.

Theorem 2.1. (Das, Gupta, and Kageyama (2002)) Suppose s_0 is an integer defined by $g(s_0; p, b, k) = \min_{1 \leq s_{d0} \leq c} g(s_{d0}; p, b, k)$, where $c = bk$ if (i) $p = 5$, $k = 3$, (ii) $p = 4$, k is odd or (iii) $p = 3$, else $c = b[k/2]$. Then a type S_0 block design $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$ with $g_0 = s_0/p$, $g_1 = (s_1 - g_0)/(p-1)$, $\lambda_0 = (2ks_0 - h(s_0))/p$, $\lambda_1 = (2ks_1 - h(s_1) - \lambda_0)/(p-1)$ and $s_1 = (2bk - s_0)/p$

is optimal in $D(p+1, b, k)$.

However, the theorem can be generalized as follows. Let $\mu_{d1} = \left(ks_{d0} - \sum_{j=1}^{b} n_{d0j}^2\right)\Big/ pk$, then in Das, Gupta, and Kageyama (2002) one has $trM_d^{-1} \geq \mu_{d1}^{-1} + (p-1)^2(2bk - s_{d0} - a(s_{d0})/k - \mu_{d1})^{-1} = \theta_d$, say.

Lemma 2.2. For given values of *p*, *b*, and *k*, suppose $d \in D(p+1, b, k)$ has $\sum_{i=1}^{p}\sum_{j=1}^{b} n_{dij}^2 = a(s_{d0})$, and $s_{d0} > b[k/2]$. Then there exists $d* \in D(p+1, b, k)$ having $\sum_{i=1}^{p}\sum_{j=1}^{b} n_{d*ij}^2 = a(s_{d*0})$ with $s_{d*0} \leq b[k/2]$, and satisfying $\theta_{d*} \leq \theta_d$ unless $p = 3$.

Proof: In the proof of Lemma 2.4 of Das, Gupta and Kageyama (2002), they set $n_{d*0j} = n_{d0j}$ if $n_{d0j} \leq [k/2]$ and $n_{d*0j} = k - n_{d0j}$ if $n_{d0j} > [k/2]$, and show that $\mu_{d1*} = \mu_{d1}$, and $2bk - s_{d0} - l(s_{d0})/k$ decreases as s_{d0} increases except when (i) p = 5, k = 3, (ii) p = 4, k odd, and (iii) p = 3. In the following, one can show that (i) and (ii) can be released.

Let $\psi(s_{d0}) = 2bk - s_{d0} - a(s_{d0})/k$. In (i), $\psi(s_{d0}) = (2/3)(6b - s_{d0})(1 - y_1) + 5by_1(y_1+1)/3$ where $y_1 = \left[(6b - s_{d0})/5b\right]$. For $0 < s_{d0} \leq b$, then $y_1 = 1$, and $\psi(s_{d0}) = 10b/3$ is a constant. For $b < s_{d0} < 6b$, then $y_1 = 0$, $\psi(s_{d0}) = 2(6b - s_{d0})/3$ is a decreasing function in s_{d0}. Moreover, $\psi(b) - \psi(b+1) = 2/3$. Hence if $s_{d0} > b[k/2] = b$, there exists a design $d*$ having $s_{d*0} \leq b$ and $\theta_{d*} \leq \theta_d$.

Similarly, in (ii), $\psi(s_{d0}) = (2b - s_{d0}/k)(k - 2y_1 - 1) + 4by_1(y_1+1)/k$, where

$y_1 = [(2bk - s_{d0})/4b] = [k/2 - s_{d0}/4b]$. For $0 < s_{d0} \le 2b$, then $y_1 = (k-1)/2$, and $\psi(s_{d0}) = b(k^2-1)/k$ is a constant. For $2b < s_{d0} < 2bk$ and fix value y_1, $\psi(s_{d0})$ is a decreasing function in s_{d0}. Moreover, denote $s' = (2+4u)b$, $s'' = (6+4u)b$, where $u \ge 0$ is an integer, then

$$y_1 = \begin{cases} (k-1)/2 - u, & \text{when } s_{d0} = s', \\ (k-3)/2 - u, & \text{when } s_{d0} = s'', \end{cases}$$

$\psi(s') - \psi(s'') = 8b(u+1)/k > 0$, and

$\psi(2b) - \psi(2b+1) = 2/k$.

Hence $\psi(s_{d0})$ is a decreasing function whenever $2b < s_{d0} < 2bk$. Thus, if $s_{d0} > b[k/2]$, there exists a design $d*$ having $s_{d*0} \le b[k/2] = b(k-1)/2$ and $\theta_{d*} \le \theta_d$.

A less restrictive and more efficient theorem, in searching for the "best" value of s_{d0}, is given in the following.

Theorem 2.3. For given values of *p*, *b*, and *k*, a type S_0 block design $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$ is A-optimal if it satisfies

(i) s_0 is a positive integer such that $g(s_0; p,b,k) = \min_{1 \le s_{d0} \le c} g(s_{d0}; p,b,k)$, where $c = bk$ if $p = 3$, else $c = b[k/2]$,

(ii) $s_1 = (2bk - s_0)/p$,

(iii) $g_0 = s_0/p$, $g_1 = (s_1 - g_0)/(p-1)$,

(iv) $\lambda_0 = (2ks_0 - h(s_0))/p$, $\lambda_1 = (2ks_1 - h(s_1) - \lambda_0)/(p-1)$.