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Optimal Designs for Best Linear Unbiased Prediction in Diallel Crosses

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Summary

Most of the available results on optimal block designs for diallel crosses are based on standard linear model assumptions where the general combining ability effects are taken as fixed. In many practical situations, this assumption may not be tenable since often one studies only a sample of inbred lines from a possibly large (hypothetical) population. Recently Ghosh and Das (2003) proposed a random effects model and then estimated the variance components and the variances of these estimates. While comparing the yielding capacities of the cross (i, j), Kempthorne and Curnow (1961) have proposed the estimation of the yielding capacity of any cross based on the least square estimators of the general combining ability effects and/or the mean yield of the cross (i, j). In this paper, the problem of predicting the yielding capacity of the cross (i, j) from the sample of inbred lines has been considered. The properties of the *best linear unbiased predictor* for predicting the unobserved general combining ability effects together with general mean effect has been studied. We characterize A-optimal complete diallel cross designs and some efficient partial diallel cross designs under this setup.

Keywords : A-optimality; BLUP; Efficient design; Partial diallel cross; Variance components.

1. Introduction

Diallel crosses as mating designs are used to study the genetic properties of inbred lines in plant breeding experiments. Plant breeders frequently need overall information on average performance of individual inbred lines in crosses for subsequent choosing the best amongst them for further breeding.

Consider a (possibly) hypothetical population involving a large number of lines and crosses so that all means are estimated without error. Crossing a line to several others provides the mean performance of the line in all its crosses. This mean performance, when expressed as a deviation from the mean of all crosses, is called the *general combining ability* (g.c.a.) of the line. Any particular cross, then, has an expected value which is the sum of the general combining abilities of its two parental lines. The cross may, however, deviate from this expected value to a greater or lesser extent. This deviation is called the *specific combining ability* (s.c.a.) of the two lines in combination. In statistical terms, the g.c.a.'s are main effects and the s.c.a. is an interaction. Griffing (1956) defines diallel crosses in terms of genotypic values where the sum of g.c.a. effects for the two gametes is the breeding value of the cross (i, j). Similarly, s.c.a. represents the dominance deviation value in the simplest case ignoring epistatic deviation; see Kempthorne (1969) and Mayo (1980) for details.

In practice, often a plant breeder carries out a diallel cross experiment by selecting p lines randomly from a population consisting of a large number of lines. In such a case, the expected value of an observation Y_{ij}, conditional on the realized value of the g.c.a. and s.c.a., arising out of cross (i, j) involving lines i and $j, i < j;\ i, j = 1, \ldots, p$ can be modeled as

$$E(Y_{ij}) = \mu + g_i^* + g_j^* + s_{ij}^* \ , \tag{1.1}$$

where μ is the general mean, g_i^* (g_j^*) is the realized value of g_i (g_j), the g.c.a. effect of sampled i-th (j-th) line and s_{ij}^* is the realized value of s_{ij}, the s.c.a. effect of cross (i, j).

Accordingly, in experimental mating design, the analysis of the observations arising out of n crosses involving p lines may be carried out based on a model

$$Y_{ijl} = \mu + g_i + g_j + e_{ijl} \ ;\ i < j, \tag{1.2}$$

where Y_{ijl} is the observation arising out of the l-th replication of the cross (i, j), g_i is the g.c.a. effect of the i-th line with $E(g_i) = 0$, $Var(g_i) = \sigma_g^2 \geq 0$, $Cov(g_i, g_j) = 0$, μ is the general mean and e_{ijl} is the random error component, uncorrelated with g_i, with expectation zero and variance $\sigma_e^2 > 0$, $1 \leq i < j \leq p$. Here μ, σ_e^2 and σ_g^2 are unknown parameters. Also, the specific combining ability effects are assumed to be negligible and have been absorbed in the error component; see Hinkelmann (1975) and Hinkelmann and Kempthorne (1963) for a discussion on this assumption. In the model (1.2), μ is a fixed effect while g_i, g_j $(i < j)$ and e_{ijl} are random effects.

An experiment is carried out using a diallel cross design with p lines and n crosses. A diallel cross experiment is said to be complete if each of the $\binom{p}{2}$ crosses appears equally often in the experiment, otherwise it is said to be a partial diallel cross experiment. Most of the available literature on optimal designs for diallel crosses is based on standard linear model assumptions where the g.c.a. effects are taken as fixed and the primary interest lies in comparing the lines with respect to their g.c.a. effects. Under such a model, among others, Gupta and Kageyama (1994), Dey and Midha (1996), Mukerjee (1997), Das, Dey and Dean (1998) and Das, Dean and Gupta (1998) have characterised and obtained optimal completely randomised designs and incomplete block designs for diallel crosses. When one is studying only a sample of inbred lines from a possibly large hypothetical population the fixed effects assumption may not be tenable. Inbred lines are often developed and then crossed in an attempt to produce crosses with a high yielding capacity where $\mu + g_i + g_j$ represents the yielding capacity of a cross (i, j). In this paper, the problem of predicting the yielding capacity of the cross (i, j) from the sample of inbred lines has been considered.

The properties of the best linear unbiased predictor (BLUP) for predicting the unobserved g.c.a. effects together with general mean effect has been studied. We first obtain the BLUP of $\mu + g_i$, $i = 1, 2, \dots, p$ and its mean square prediction error. Then we characterize A-optimal complete diallel cross designs and some efficient partial diallel cross designs.

2. BLUP of g.c.a. Effects And Optimal Diallel Cross Designs

The starting point is the traditional fixed effects linear model written as

$$y = X\boldsymbol{\beta} + e \tag{2.1}$$

where y is $N \times 1$ vector of observations, $\boldsymbol{\beta}$ is a $p \times 1$ vector of fixed effects parameters, X is the $N \times p$ incidence matrix and e is an error vector defined as $e = y - I\!E(y) = y - X\boldsymbol{\beta}$ and thus has $I\!E(e) = 0$. To e is usually attributed the dispersion matrix $I\!D(e) = \sigma_e^2 I_N$. Here I_t denotes an identity matrix of order t. In situations where the order is evident from the context, we write I instead of I_t. In variance components model the random effects of a model can be represented as $Z\boldsymbol{u}$ (of a nature that parallels $X\boldsymbol{\beta}$), where $\boldsymbol{u}$ is the vector of the random effects that occur in modelling an observation, and Z the corresponding matrix, usually an incidence matrix. Moreover, $\boldsymbol{u}$ can be partitioned into a series of r sub-vectors.

$$\boldsymbol{u} = \left[\boldsymbol{u}_1' \; \boldsymbol{u}_2' \; \ldots \; \boldsymbol{u}_r'\right]'. \tag{2.2}$$

Incorporating $\boldsymbol{u}$ of (2.2) into $y = X\boldsymbol{\beta} + e$ gives a general form of model equation for a mixed model as

$$y = X\boldsymbol{\beta} + Z\boldsymbol{u} + e \tag{2.3}$$

with $\boldsymbol{\beta}$ and $\boldsymbol{u}$ representing fixed and random effects respectively.

To $\boldsymbol{u}$ we now attribute the usual variance-covariance structure, i.e.,

$$I\!D(\boldsymbol{u}_i) = \sigma_i^2 I_{q_i} \text{ for } i = 1, \ldots, r \tag{2.4}$$

$$\text{Cov}(\boldsymbol{u}_i, \boldsymbol{u}_j) = 0 \text{ for } i \neq j, \tag{2.5}$$

and similarly for all elements of $\boldsymbol{u}$ and e, $\text{Cov}(\boldsymbol{u}, e) = 0$.

Utilizing (2.2)-(2.5), the mean and variance structures of $\boldsymbol{u}$ are $\mu_{\boldsymbol{u}} = I\!E(\boldsymbol{u}) = 0$, and

$$I\!D(\boldsymbol{u}) = \begin{bmatrix} \sigma_1^2 I_{q_1} & 0 & \cdots & 0 \\ 0 & \sigma_2^2 I_{q_2} & & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & \sigma_r^2 I_{q_r} \end{bmatrix}.$$

Then partitioning Z conformably with $\boldsymbol{u}$ of (2.2) as $Z = [Z_1 \; Z_2 \; \ldots \; Z_r]$ gives

$$y = X\boldsymbol{\beta} + Z\boldsymbol{u} + e = X\boldsymbol{\beta} + \sum_{i=1}^{r} Z_i \boldsymbol{u}_i + e. \tag{2.6}$$

Hence

$$\mu_y = I\!E(y) = X\boldsymbol{\beta}, \; V_y = I\!D(y) = Z I\!D(\boldsymbol{u}) Z' + \sigma_e^2 I = \sum_{i=1}^{r} \sigma_i^2 Z_i Z_i' + \sigma_e^2 I \tag{2.7}$$

and

$$C_{uy} = \text{ Cov }(\boldsymbol{u}, y) = I\!D(\boldsymbol{u}) Z'. \tag{2.8}$$

In case of mixed model prediction, we consider the problem of predicting

$$\boldsymbol{w} = L'\boldsymbol{\beta} + \boldsymbol{u} \tag{2.9}$$

for some known matrix L, such that $L'\boldsymbol{\beta}$ is estimable, i.e., $L' = T'X$ for some matrix T. Since $\boldsymbol{w}$ involves both fixed effects and random effects, we will 'predict' $\boldsymbol{w}$, and will choose $\widetilde{\boldsymbol{w}}$ as the Best Predictor having the following three properties:

$$\text{“Best” in the sense of minimizing } I\!E(\boldsymbol{w} - \widetilde{\boldsymbol{w}})'A(\boldsymbol{w} - \widetilde{\boldsymbol{w}}), \text{ for some p.d. matrix } A \tag{2.10}$$

$$\text{Linear in } y : \widetilde{\boldsymbol{w}} = \boldsymbol{a} + By, \text{ with } \boldsymbol{a} \text{ and } B \text{ not involving } \boldsymbol{\beta} \tag{2.11}$$

$$\text{Unbiased } : I\!E(\widetilde{\boldsymbol{w}}) = I\!E(\boldsymbol{w}) \tag{2.12}$$

The unbiasedness of $\widetilde{\boldsymbol{w}}$ in (2.12) demands that $\boldsymbol{a} + BX\boldsymbol{\beta} = L'\boldsymbol{\beta}$ for all $\boldsymbol{\beta}$, and if $\boldsymbol{a}$ is not to depend on $\boldsymbol{\beta}$ then $\boldsymbol{a} = 0$ and $BX = L'$.

It can be shown that (see Searle et al., 1992, page 270)

$$BLUP(\boldsymbol{w}) = \widetilde{\boldsymbol{w}} = L'\boldsymbol{\beta}^\circ + C_{uy}V_y^{-1}(y - X\boldsymbol{\beta}^\circ) \tag{2.13}$$

with

$$BLUE(X\boldsymbol{\beta}) = X\boldsymbol{\beta}^\circ = X(X'V_y^{-1}X)^- X'V_y^{-1}y. \tag{2.14}$$

We shall make the same assumption and use the same notation as above, while obtaining best linear unbiased predictor of g.c.a. effects. When a complete diallel cross experiment is not possible due to limitations of experimental units, one may consider a partial diallel cross, with some unobserved crosses, as a method for predicting the yielding capacities of all the possible single crosses among p inbred lines. The yielding capacity of all crosses in the diallel cross including the unsampled crosses whose yields are not observed in case of partial diallel cross can be predicted in two ways. Firstly, they can be predicted by their mean yields in the experiment when the yield of the crosses are observed in the experiment. Secondly, specific combining ability can be ignored and the yielding capacity of the cross (i, j) is estimated by $\hat{\mu} + \hat{g}_i + \hat{g}_j$ where $\hat{g}_i$ is some predicted value of g.c.a. effect g_i, both for sampled crosses as well as unsampled crosses. Kempthorne and Curnow (1961) have designated the methods of estimation A and B, where A and B are defined as follows:

[A.] Unsampled crosses estimated by $\hat{\mu} + \hat{g}_i + \hat{g}_j$ but sampled crosses estimated by cross means $\bar{y}_{ij\cdot}$.

[B.] Both unsampled and sampled crosses estimated by $\hat{\mu} + \hat{g}_i + \hat{g}_j$.

We show that, in general, method B will perform better than method A when the $\hat{g}_i$'s are chosen by the method of BLUP.

When an experiment is carried out using unblocked diallel cross design (d) with p lines and n crosses, we can represent the model in matrix notation as

$$Y = \mu 1_n + D_1'g + e \tag{2.15}$$

where Y is the vector of n observation, g is the $p \times 1$ vector of general combining ability effects with $\mathbb{E}(g) = 0$ and $\mathbb{D}(g) = \sigma_g^2 I_p$, e is the error vector with $\mathbb{E}(e) = 0$ and $\mathbb{D}(e) = \sigma_e^2 I_n$, and $D_1 = (d_{uv}^{(1)})$ is the $p \times n$ line versus observation incidence matrix with $d_{uv}^{(1)} = 1$ if v-th observation is out of a cross involving uth line and $d_{uv}^{(1)} = 0$ otherwise. Here 1_t represents a $t \times 1$ column vector of all ones and in situation where the order is evident from the context, we write 1 instead of 1_t. Equivalently (2.15) can be written as $Y = X\mu + Z\boldsymbol{u} + e$ where $X = 1_n$, $Z = D_1'$, $\boldsymbol{u} = g$. Here,

$$\mathbb{E}(Y) = \mu 1_n, \quad \mathbb{D}(Y/\sigma_g^2, \sigma_e^2) = \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n \tag{2.16}$$

Also,

$$\text{Cov}\,(g, Y) = \text{Cov}\,(g, \mu 1_n + D_1' g + e) = \sigma_g^2 D_1. \tag{2.17}$$

We consider the problem of predicting $\boldsymbol{w} = L'\mu + g$ where $L' = 1_p$.

Then, as described in equations (2.9)-(2.14), the Best Linear Unbiased Predictor of $\boldsymbol{w}$ is

$$\widetilde{\boldsymbol{w}} = BLUP(\boldsymbol{w}) = L'\mu^0 + CV^{-1}(Y - \mu^0 1_n) \tag{2.18}$$

where μ^0 is the GLSE of μ, $C = \sigma_g^2 D_1$ and $V = \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n$. Also define $D = \mathbb{D}(g) = \sigma_g^2 I_p$. Let $\mathcal{D}(p, n)$ be a class of unblocked diallel cross designs involving p inbred lines and n crosses. Given a design $d \in \mathcal{D}(p, n)$, the minimum mean square prediction error is

$$\begin{aligned} MSE(BLUP(\boldsymbol{w}), d) &= \mathbb{E}\left[(\widetilde{\boldsymbol{w}} - \boldsymbol{w})'(\widetilde{\boldsymbol{w}} - \boldsymbol{w})\right] = \mathbb{E}\left[\text{tr}\,(\widetilde{\boldsymbol{w}} - \boldsymbol{w})(\widetilde{\boldsymbol{w}} - \boldsymbol{w})'\right] \\ &= \text{tr}\,\mathbb{E}\left[(\widetilde{\boldsymbol{w}} - \boldsymbol{w})(\widetilde{\boldsymbol{w}} - \boldsymbol{w})'\right] = \text{tr}\,\mathbb{D}\left[\widetilde{\boldsymbol{w}} - \boldsymbol{w}\right]. \end{aligned} \tag{2.19}$$

Clearly, $MSE(BLUP(\boldsymbol{w}), d)$ depends on the design d. A design $d^* \in \mathcal{D}(p, n)$ will be called A-optimal over $\mathcal{D}(p, n)$ if

$$MSE(BLUP(\boldsymbol{w}), d^*) = \min_{d \in \mathcal{D}(p,n)} MSE(BLUP(\boldsymbol{w}), d). \tag{2.20}$$

Now, using the properties of BLUP given in Searle et al. (1992, page 272) we observe that,

$$\begin{aligned}
&\text{tr}\,\mathbb{D}\left[\widetilde{\boldsymbol{w}} - \boldsymbol{w}\right] \\
&= \text{tr}\,\mathbb{D}\left[(L'\mu^0 - L'\mu) + (g^0 - g)\right] \quad \text{where } g^0 = CV^{-1}(Y - \mu^0 1_n) \\
&= \text{tr}\,\Big[\mathbb{E}(L'\mu^0 - L'\mu)(L'\mu^0 - L'\mu)' + \mathbb{E}(g^0 - g)(g^0 - g)' \\
&\quad + \mathbb{E}(L'\mu^0 - L'\mu)(g^0 - g)' + \mathbb{E}(g^0 - g)(L'\mu^0 - L'\mu)'\Big]. \\
&= \text{tr}\,\mathbb{D}(L'\mu^0) + \text{tr}\,\mathbb{D}(g^0 - g) \\
&\quad + 2\text{tr}\,\text{Cov}\,(L'\mu^0, g^0 - g), \quad \text{since } \text{tr}\,\text{Cov}\,(X, Y) = \text{tr}\,\text{Cov}\,(Y, X) \\
&= \text{tr}\,\mathbb{D}(L'\mu^0) + \text{tr}\,\mathbb{D}(g^0 - g) - 2\,\text{tr}\,\text{Cov}\,(L'\mu^0, g), \quad \text{since } \text{Cov}\,(L'\mu^0, g^0) = 0 \\
&= \text{tr}\left[L'(X'V^{-1}X)^- L\right] + \text{tr}\left[D - \mathbb{D}(g^0)\right] \\
&\quad - 2\,\text{tr}\left[L'(X'V^{-1}X)^- X'V^{-1}C'\right], \text{ since } \mathbb{D}(L'\mu^0) = L'(X'V^{-1}X)^- L, \\
&\qquad\qquad \mathbb{D}(g^0 - g) = D - \mathbb{D}(g^0) \\
&\qquad\qquad \text{and } \text{Cov}\,(L'\mu^0, g) = L'(X'V^{-1}X)^- X'V^{-1}C'
\end{aligned}$$

$$= \text{tr}\,\left[L'(X'V^{-1}X)^{-}L\right] + \text{ tr}\,D - \text{ tr}\left[CV^{-1}C'\right] + \text{ tr}\,\left[CV^{-1}X(X'V^{-1}X)^{-}X'V^{-1}C'\right]$$
$$- 2\text{tr}\left[L'(X'V^{-1}X)^{-}X'V^{-1}C'\right]. \tag{2.21}$$

Here tr$(\cdot)$ denotes the trace of a square matrix. The first term in (2.21) simplifies to

$$\text{tr}\,\left[L'(X'V^{-1}X)^{-}L\right] = \text{ tr}\,\left[1(1'V^{-1}1)^{-1}1'\right] = \frac{p}{1'V^{-1}1}. \tag{2.22}$$

We now give a standard matrix result.

Lemma 2.1 Let A and B be two non negative definite matrices each of order p, such that $AB = BA$. Then there exists an orthogonal matrix $P = (l_1, l_2, \ldots, l_p)$ such that $P'AP = D_1$, $P'BP = D_2$ where $D_1 = \text{diag}(\lambda_1^{(1)}\lambda_2^{(1)}\ldots\lambda_p^{(1)})$ and $D_2 = \text{diag}(\lambda_1^{(2)}\lambda_2^{(2)}\ldots\lambda_p^{(2)})$, $\lambda_i^{(1)}, i = 1, \ldots, p$ are the eigenvalues of A and $\lambda_i^{(2)}, i = 1, \ldots, p$ are the eigenvalues of B. Also, $Al_i = \lambda_i^{(1)}l_i$ and $Bl_i = \lambda_i^{(2)}l_i, i = 1, \ldots, p$ or equivalently $(A + B)l_i = (\lambda_i^{(1)} + \lambda_i^{(2)})l_i, i = 1, \ldots, p.$

Since the matrix V involves $D_1'D_1$, to obtain eigen vectors of $D_1'D_1$ orthogonal to the vector 1, we restrict the class of design to $\mathcal{D}_0(p, n) = \{d : s_{d1} = s_{d2} = \cdots = s_{dp} = s\}$ where s_{di} = number of times ith line being appeared in the design d.

Then $D_1'D_1 1 = D_1's1 = 2s1$. Hence using Lemma 2.1 we get $\sigma_g^2 D_1'D_1\frac{1}{\sqrt{n}} = (2s\sigma_g^2)\frac{1}{\sqrt{n}}$ i.e., $(\sigma_g^2 D_1'D_1 + \sigma_e^2 I_n)\frac{1}{\sqrt{n}} = (2s\sigma_g^2 + \sigma_e^2)\frac{1}{\sqrt{n}}$ which means $l_1 = \frac{1}{\sqrt{n}}$ is an eigen vector corresponding to eigenvalue $\lambda_1 = (2s\sigma_g^2 + \sigma_e^2)$. Let $l_2, l_3, \ldots, l_n$ be the other $(n-1)$ orthonormal eigen vectors of V corresponding to eigenvalues $\lambda_2, \lambda_3, \ldots, \lambda_n$. Then,

$$1'V^{-1}1 = 1'\left[(2s\sigma_g^2 + \sigma_e^2)^{-1}\frac{1}{\sqrt{n}}\frac{1'}{\sqrt{n}} + \sum_{i=2}^{n}\lambda_i^{-1}l_il_i'\right]1 = n(2s\sigma_g^2 + \sigma_e^2)^{-1}. \tag{2.23}$$

Then, combining (2.22) and (2.23) we get

$$\text{tr}\,\left[L'(X'V^{-1}X)^{-}L\right] = \frac{p(2s\sigma_g^2 + \sigma_e^2)}{n}. \tag{2.24}$$

The second term in (2.21) is

$$\text{tr}\,D = \text{ tr}\,\sigma_g^2 I_p = p\sigma_g^2 \tag{2.25}$$

and the third term in (2.21) is

$$\begin{aligned} -\text{tr}\,CV^{-1}C' &= -\text{tr}\,\sigma_g^2 D_1 V^{-1}\sigma_g^2 D_1' = -\sigma_g^4 \text{tr}\,D_1V^{-1}D_1' = -\sigma_g^4\,\text{tr}\,D_1'D_1V^{-1} \\ &= -\sigma_g^4\,\text{tr}\,\left[V - \sigma_e^2 I_n\right]V^{-1} = -\sigma_g^2\,\text{tr}\,\left[I_n - \sigma_e^2 V^{-1}\right] \\ &= -\sigma_g^2\left[n - \sigma_e^2\left(\frac{1}{2s\sigma_g^2 + \sigma_e^2}\right) - \sigma_e^2\sum_{i=2}^{n}\frac{1}{\lambda_i}\right]. \end{aligned} \tag{2.26}$$

Note that the non zero eigenvalues of $D_1'D_1$ are the non zero eigenvalues of $D_1D_1' = G$ which are $\lambda_{G1} = 2s, \lambda_{G2}, \ldots, \lambda_{Gp}$. Then $\lambda_i = \sigma_g^2\lambda_{Gi} + \sigma_e^2,$ for $i = 2, \ldots, p$ and $\lambda_i = \sigma_e^2$ for $i = (p+1), \ldots, n,$

and, (2.26) reduces to

$$-\sigma_g^2\left[n-\sigma_e^2\left(\frac{1}{2s\sigma_g^2+\sigma_e^2}\right)-\sum_{i=2}^{p}\frac{\sigma_e^2}{\sigma_g^2\lambda_{Gi}+\sigma_e^2}-\sigma_e^2\sum_{i=p+1}^{n}\frac{1}{\sigma_e^2}\right]$$

$$= \quad -\sigma_g^2\left[n-\sigma_e^2\left(\frac{1}{2s\sigma_g^2+\sigma_e^2}\right)-\sum_{i=2}^{p}\frac{\sigma_e^2}{\sigma_g^2\lambda_{Gi}+\sigma_e^2}-(n-p)\right]$$

$$=-\sigma_g^2\left[p-\sigma_e^2\left(\frac{1}{2s\sigma_g^2+\sigma_e^2}\right)-\sum_{i=2}^{p}\frac{\sigma_e^2}{\sigma_g^2\lambda_{Gi}+\sigma_e^2}\right]. \tag{2.27}$$

Using (2.23), the fourth term in (2.21) reduces to

$$\text{tr }\left[CV^{-1}X(X'V^{-1}X)^{-}X'V^{-1}C'\right]=\text{tr }\left[\sigma_g^2D_1V^{-1}1(1'V^{-1}1)^{-}1'V^{-1}\sigma_g^2D_1'\right]$$

$$= \quad \sigma_g^4\text{ tr }\left[D_1'D_1V^{-1}11'(2s\sigma_g^2+\sigma_e^2)^{-1}\frac{1\,1'}{n}\right]\Big/(1'V^{-1}1)=\frac{\sigma_g^4(2s\sigma_g^2+\sigma_e^2)}{n(2s\sigma_g^2+\sigma_e^2)}\text{ tr }\left[D_1'D_1V^{-1}11'\right]$$

$$= \quad \frac{\sigma_g^4}{n}\text{ tr }\left[\frac{1}{\sigma_g^2}(V-\sigma_e^2I_n)V^{-1}11'\right]=\frac{\sigma_g^2}{n}\text{ tr }\left[(I-\sigma_e^2V^{-1})11'\right]=\frac{\sigma_g^2}{n}\left[n-\text{ tr }\sigma_e^21'V^{-1}1\right]$$

$$= \quad \frac{\sigma_g^2}{n}\left[n-\sigma_e^2\frac{n}{2s\sigma_g^2+\sigma_e^2}\right],$$

i.e.,

$$\text{tr }\left[\sigma_g^2D_1V^{-1}1(1'V^{-1}1)^{-}1'V^{-1}\sigma_g^2D_1'\right]=\sigma_g^2-\frac{\sigma_g^2\sigma_e^2}{2s\sigma_g^2+\sigma_e^2}=\frac{2s\sigma_g^4}{2s\sigma_g^2+\sigma_e^2}. \tag{2.28}$$

Finally, the fifth term in (2.21) is

$$-2\text{tr }\left[L'(X'V^{-1}X)^{-}X'V^{-1}C'\right]=-2\text{tr }\left[1(1'V^{-1}1)^{-}1'V^{-1}\sigma_g^2D_1'\right]$$

$$=-2\sigma_g^2\left[1'V^{-1}D_1'1\right]/(1'V^{-1}1)=-2\sigma_g^2\left[21'V^{-1}1\right]/(1'V^{-1}1),$$

i.e.,

$$-2\text{tr }\left[L'(X'V^{-1}X)^{-}X'V^{-1}C'\right]=-4\sigma_g^2. \tag{2.29}$$

Using (2.21)-(2.29) we get

$$MSE(BLUP(\boldsymbol{w}),d)=\frac{(2ps-3n)\sigma_g^2+p\sigma_e^2}{n}+\sigma_e^2\sum_{i=2}^{p}\frac{1}{\lambda_{Gi}+\frac{\sigma_e^2}{\sigma_g^2}}. \tag{2.30}$$

Theorem 2.1 The design d^* with $\lambda_{G_{d^*}i}=\lambda$, $i=2,\ldots,p$ is A-optimal in $\mathcal{D}_0(p,n)$ for Best Linear Unbiased Prediction of $\boldsymbol{w}=L'\mu+g$, where $L'=1_p$ and g is $p\times 1$ vector of g.c.a. effects.

Proof. From (2.30) we observe that it is enough to minimize $\sum_{i=2}^{p}\frac{1}{\lambda_{G_di}+\frac{\sigma_e^2}{\sigma_g^2}}$ which is equivalent to minimizing $\sum_{i=2}^{p}\frac{1}{\lambda^*_{G_di}}$ where $\lambda^*_{G_di}=\lambda_{G_di}+\frac{\sigma_e^2}{\sigma_g^2}$.

Now, from $AM - HM$ inequality we have, $\frac{\sum_{i=1}^{n} x_i}{n} \geq \frac{n}{\sum_{i=1}^{n} x_i^{-1}}$ where $x_1, x_2, \ldots, x_n$ are n positive real numbers. That is $\sum_{i=1}^{n} \frac{1}{x_i} \geq \frac{n^2}{\sum_{i=1}^{n} x_i}$, equality being attained when $x_1 = x_2 = \cdots = x_n = x$.

Now $\sum_{i=1}^{p} \lambda^*_{G_d i} =$ tr $G_d + p\frac{\sigma_e^2}{\sigma_g^2} = 2n + p\frac{\sigma_e^2}{\sigma_g^2}$ and $\lambda_{G_d 1} = 2s$ which implies $\sum_{i=2}^{p} \lambda^*_{G_d i} = 2n - 2s + (p-1)\frac{\sigma_e^2}{\sigma_g^2} = 2(n-s) + (p-1)\frac{\sigma_e^2}{\sigma_g^2}$.

Hence,

$$\sum_{i=2}^{p} \frac{1}{\lambda^*_{G_d i}} \geq \frac{(p-1)^2}{2(n-s) + (p-1)\frac{\sigma_e^2}{\sigma_g^2}}, \tag{2.31}$$

equality being attained if and only if $\lambda^*_{G_d 2} = \lambda^*_{G_d 3} = \cdots = \lambda^*_{G_d p} = \lambda^*$ which is equivalent to $\lambda_{G2} = \lambda_{G3} = \cdots = \lambda_{Gp} = \lambda$.

Corollary 2.1 The design d^* with a completely symmetric G-matrix is A-optimal in $\mathcal{D}_0(p,n)$ for Best Linear Unbiased Prediction of g.c.a. effects. Equivalently, a complete diallel cross design with p lines and n crosses is A-optimal in $\mathcal{D}_0(p,n)$.

3. Efficient Partial Diallel Cross Designs

In case of partial diallel cross experiment where $n < \binom{p}{2}$, the optimal diallel cross design which minimizes $MSE(BLUP(\boldsymbol{w}), d)$ over the class $\mathcal{D}_0(p,n) = \{d : s_{d1} = s_{d2} = \cdots = s_{dp} = s\}$, is not straightforward to identify as compared to that of complete diallel cross experiment. Mukerjee (1997) has investigated the optimality of certain partial diallel crosses, under fixed effects model, which are linked with a certain class of group divisible designs. Though his results are on E-optimality, he also presented results on A-optimality in the saturated case. In general, the E-optimal designs turn out to be highly efficient under the D- and A-optimality criteria.

Let $p = n_1 n_2$ where $n_1 \geq 2$, $n_2 \geq 3$. Partition the set $\{1, 2, \ldots, p\}$ into n_1 mutually exclusive and exhaustive subsets $\{S_1, S_2, \ldots, S_{n_1}\}$ each of cardinality n_2. Let

$$d^* = \{(i,j) : 1 \leq i < j \leq p \text{ and } i,j \in S_u \text{ for some } u\}. \tag{3.1}$$

Then $d^* \in \mathcal{D}(n_1 n_2, \frac{1}{2} n_1 n_2 (n_2 - 1))$. From Mukerjee (1997), for $i = 1, \ldots, n_1(n_2-1)$, $\lambda_{d^* i} = n_2 - 2$ and for $i = n_1(n_2-1)+1, \ldots, n_1 n_2 - 1$, $\lambda_{d^* i} = 2(n_2-1)$. Now since d^* is E-optimal in $\mathcal{D}(n_1 n_2, \frac{1}{2} n_1 n_2 (n_2-1))$ the following holds:

$$\lambda_{d1} \leq \lambda_{d^* 1} = n_2 - 2, \text{ for } d \in \mathcal{D}(n_1 n_2, \frac{1}{2} n_1 n_2 (n_2 - 1)). \tag{3.2}$$

Here $\lambda_{d1} \leq \lambda_{d2} \leq \cdots \leq \lambda_{d(p-1)}$ are the non zero eigenvalues of the information matrix $C_d = G_d - \frac{1}{n} s_d s_d'$, $s_d = (s_{d1}, s_{d2}, \ldots, s_{dp})$, $p = n_1 n_2$, $n = \frac{1}{2} n_1 n_2 (n_2 - 1)$. Also, the design d^* is A-optimal if and only if $\sum_{i=1}^{p-1} \frac{1}{\lambda_{d^* i}} = \min_{d \in \mathcal{D}(p,n)} \sum_{i=1}^{p-1} \frac{1}{\lambda_{di}}$.

Now it is easy to see that $d^* \in \mathcal{D}_0(p,n)$ and the non zero eigenvalues λ_{di} of C_d, $1 \leq i \leq p-1$, are the same as the eigenvalues $\lambda_{G_d i}$ of G_d, $2 \leq i \leq p$ where $d \in \mathcal{D}_0(p,n)$.

Thus, using (2.31), a lower bound to $\sum_{i=2}^{p}\frac{1}{\lambda_{G_d i}+\frac{\sigma_e^2}{\sigma_g^2}}$ for $d \in \mathcal{D}_0(p,n)$ is given by

$$\sum_{i=2}^{p}\frac{1}{\lambda_{G_d i}+\frac{\sigma_e^2}{\sigma_g^2}} \geq \frac{(p-1)^2}{2(n-s)+(p-1)\frac{\sigma_e^2}{\sigma_g^2}} \tag{3.3}$$

where $s = n_2 - 1$.

The lower bound in (3.3) will be attained only when $\lambda_{G_d 2} = \lambda_{G_d 3} = \cdots = \lambda_{G_d p} = \frac{2(n-s)}{p-1}$ i.e. d is a complete diallel cross design. But $\frac{2(n-s)}{p-1} = \frac{(n_2-1)(p-2)}{p-1} = (n_2-1) - \frac{n_2-1}{p-1} > n_2 - 2$ which is not possible since from (3.2) it follows that $\lambda_{G_d 2} \leq n_2 - 2$ where $\lambda_{G_d 2} \leq \cdots \leq \lambda_{G_d p}$ and $d \in \mathcal{D}_0(p,n)$. Based on this fact the following theorem establishes a sharper lower bound for $\sum_{i=2}^{p}\frac{1}{\lambda_{G_d i}+\frac{\sigma_e^2}{\sigma_g^2}}$.

Theorem 3.1 Given the class $\mathcal{D}_0(p,n)$ of partial diallel cross designs, where $p = n_1 n_2$, $n = \frac{1}{2}n_1 n_2(n_2-1)$, and $s_{d1} = s_{d2} = \cdots = s_{dp} = n_2 - 1$,

$$\sum_{i=2}^{p}\frac{1}{\lambda_{G_d i}+\frac{\sigma_e^2}{\sigma_g^2}} \geq \frac{1}{n_2-2+\frac{\sigma_e^2}{\sigma_g^2}} + \frac{(p-2)^2}{(n_2-1)(p-3)+1+(p-2)\frac{\sigma_e^2}{\sigma_g^2}} \quad (= L(n_1, n_2, \frac{\sigma_e^2}{\sigma_g^2}),\ \text{say}) \tag{3.4}$$

for all $d \in \mathcal{D}_0(p,n)$.

Proof. Writing $\lambda_{G_d i} = \lambda_i$, we obtain

$$\begin{aligned}
\sum_{i=2}^{p}\frac{1}{\lambda_i+\frac{\sigma_e^2}{\sigma_g^2}} &= \frac{1}{\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}} + \sum_{i=3}^{p}\frac{1}{\lambda_i+\frac{\sigma_e^2}{\sigma_g^2}} \\
&\geq \frac{1}{\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}} + \frac{(p-2)^2}{\sum_{i=2}^{p}\lambda_i+\frac{\sigma_e^2}{\sigma_g^2}(p-1)-\lambda_2-\frac{\sigma_e^2}{\sigma_g^2}}, \ \text{by AM-HM inequality} \\
&= \frac{1}{\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}} + \frac{(p-2)^2}{(n_2-1)(p-2)-\lambda_2+(p-2)\frac{\sigma_e^2}{\sigma_g^2}}, \ \text{since } \sum_{i=2}^{p}\lambda_i = (n_2-1)(p-2)
\end{aligned}$$

Let $f(\lambda_2) = \frac{1}{\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}} + \frac{(p-2)^2}{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2}$. Then

$$\begin{aligned}
f'(\lambda_2) &= -\frac{1}{\left(\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}\right)^2} + \frac{(p-2)^2}{\left\{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2\right\}^2} = 0 \\
&\Leftrightarrow \frac{(p-2)^2\left(\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}\right)^2 - \left\{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2\right\}^2}{\left\{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2\right\}^2\left(\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}\right)^2} = 0 \\
&\Leftrightarrow \left\{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2+(p-2)\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}(p-2)\right\} \\
&\qquad \left\{(p-2)\lambda_2+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-(n_2-1)(p-2)-(p-2)\frac{\sigma_e^2}{\sigma_g^2}+\lambda_2\right\} = 0 \\
&\Leftrightarrow \left\{(n_2-1)(p-2)+(p-3)\lambda_2+2(p-2)\frac{\sigma_e^2}{\sigma_g^2}\right\}\{(p-1)\lambda_2-(n_2-1)(p-2)\} = 0
\end{aligned}$$

Thus, the possible stationary values of the function $f(\lambda_2)$ are $-\frac{p-2}{p-3}\left[2\frac{\sigma_e^2}{\sigma_g^2}+n_2-1\right]$ and $\frac{(n-1)(p-2)}{p-1}$ out of which only the second one is admissible.

Now,

$$f'(\lambda_2) = \frac{(p-3)(p-1)\left[\lambda_2+\frac{p-2}{p-3}\left\{n_2-1+2\frac{\sigma_e^2}{\sigma_g^2}\right\}\right]\left[\lambda_2-\frac{(n_2-1)(p-2)}{p-1}\right]}{\left\{(n_2-1)(p-2)+(p-2)\frac{\sigma_e^2}{\sigma_g^2}-\lambda_2\right\}^2\left(\lambda_2+\frac{\sigma_e^2}{\sigma_g^2}\right)^2}$$

is negative when $0<\lambda_2<\frac{(n_2-1)(p-2)}{p-1}$ and positive when $\lambda_2>\frac{(n_2-1)(p-2)}{p-1}$.

Thus $f(\lambda_2)$ is a decreasing function for $0<\lambda_2<\frac{(n_2-1)(p-2)}{p-1}$ and since $\lambda_2=\frac{(n_2-1)(p-2)}{p-1}>n_2-2$, from (3.2), the minima is attained at $\lambda_2=n_2-2$. Hence a sharper lower bound for $f(\lambda_2)$ is

$$f(n_2-2)=\frac{1}{n_2-2+\frac{\sigma_e^2}{\sigma_g^2}}+\frac{(p-2)^2}{(n_2-1)(p-3)+1+(p-2)\frac{\sigma_e^2}{\sigma_g^2}}.$$

From (2.30) and (3.4), taking into account the given values of σ_g^2, σ_e^2, the efficiency of the design $d^*\in\mathcal{D}_0(p,n)$ due to MSE(BLUP($\boldsymbol{w}$), d^*) is at least as large as $e_{BLUP}(n_1,n_2)$ where

$$e_{BLUP}(n_1,n_2)=\frac{n^{-1}\{(2ps-3n)\frac{\sigma_g^2}{\sigma_e^2}+p\}+L(n_1,n_2,\frac{\sigma_e^2}{\sigma_g^2})}{n^{-1}\{(2ps-3n)\frac{\sigma_g^2}{\sigma_e^2}+p\}+\sum_{i=2}^{p}\{\lambda_{G_{d^*}i}+\frac{\sigma_e^2}{\sigma_g^2}\}^{-1}},$$

i.e. substituting the values of $\lambda_{G_{d^*}i}$, we have

$$e_{BLUP}(n_1,n_2)=\frac{n^{-1}\{(2ps-3n)\frac{\sigma_g^2}{\sigma_e^2}+p\}+L(n_1,n_2,\frac{\sigma_e^2}{\sigma_g^2})}{n^{-1}\{(2ps-3n)\frac{\sigma_g^2}{\sigma_e^2}+p\}+n_1s\{n_2-2+\frac{\sigma_e^2}{\sigma_g^2}\}^{-1}+(n_1-1)\{2s+\frac{\sigma_e^2}{\sigma_g^2}\}^{-1}}. \quad (3.5)$$

The efficiency lower bound $e_{BLUP}(n_1,n_2)$ has been obtained for the designs in the practical range $n_1\geq 2, n_2\geq 3, p\leq 30$ and $0.01\leq\sigma_e^2/\sigma_g^2\leq 1$ with increments of 0.01. Of the 3800 possible cases, 99.6%, 91%, 77.8% and 51.9% of the designs have e_{BLUP} greater than 0.8, 0.85, 0.9 and 0.95 respectively. Also, if we restrict to designs having $n_1\leq n_2$ then of the 2700 possible cases, 100%, 100%, 98% and 72.1% of the designs have e_{BLUP} greater than 0.8, 0.85, 0.9 and 0.95 respectively. For the sake of brevity, these efficiencies for the designs are not tabulated here and they will be reported elsewhere.

Finally, note that Mukerjee (1997) has shown the A-optimality of d^* for $n_2=3$. Also, $\sum_{i=2}^{p}\{\lambda_{G_{d^*}i}+\frac{\sigma_e^2}{\sigma_g^2}\}^{-1}$ considered as a function of $\frac{\sigma_e^2}{\sigma_g^2}$ is continuous. Thus it can be shown that there exists a neighbourhood $\mathcal{N}_0$, say, at $\sigma_e^2/\sigma_g^2=0$ for which d^* is A-optimal in $\mathcal{D}_0(3n_1,3n_1)$.

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