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Estimation of ratio of variance components and optimal diallel cross designs

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Abstract

The results on optimal designs for diallel crosses are based on standard linear model assumptions where the general combining ability effects are taken as fixed. Recently Ghosh and Das (2003) proposed a random effects model that allows one to first estimate the variance components and then obtain the variances of these estimates. In this paper we first propose an unbiased estimate of the ratio of the variance components which has a one-to-one relation with heritability. We then obtain a large sample expression of the variance of this unbiased estimator of the ratio of variance components. Through a simulation study, it is shown that even for small samples, the large sample variance is close to the exact variance. Through minimization of the large sample variance we obtain optimal designs and show certain connections with the optimization problem under the fixed effects model.

Keywords : A-optimality, Variance components, Heritability, Asymptotically unbiased estimate, Large sample variance.

1. Introduction

Plant breeders frequently need overall information on average performance of individual inbred lines in crosses known as general combining ability. For this purpose diallel crossing techniques are employed. Griffing (1956) defines a model for diallel crosses in terms of genotypic values where the breeding value of the cross (i,j) is expressed as the sum of general combining abilities for the two lines. In certain contexts, specific combining ability effects representing the interaction between lines i and j in a cross (i,j) are also included in the model; see Kempthorne (1969) and Mayo (1980) for details.

Accordingly the analysis of the observations arising out of n crosses involving p lines is carried out by postulating a model

$$Y_{ijl} = \mu + g_i + g_j + e_{ijl} \; ; \; i < j, \tag{1.1}$$

where Y_{ijl} is the observation arising out of the l-th replication of the cross (i,j), g_i is the i-th line effect 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 $\sigma_e^2 > 0$, $1 \le i < j \le p$. 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. In the model, (1.2), μ is a fixed effect while g_i, g_j ($i < j$) and e_{ijl} are random effects.

Our primary interest is in *heritability* which is defined as $h^2 = 4\sigma_g^2/(2\sigma_g^2 + \sigma_e^2)$. Such a measure expresses the extent to which individual's phenotypes are determined by genotypes. In order to get a good estimate of h^2 we propose optimal designs for unbiased estimation of σ_g^2/σ_e^2 since $h^2 = \frac{4\sigma_g^2}{2\sigma_g^2+\sigma_e^2} = \frac{4(\sigma_g^2/\sigma_e^2)}{2(\sigma_g^2/\sigma_e^2)+1}$. Let T be an unbiased estimator of σ_g^2/σ_e^2. Then an estimator of h^2 is $\frac{4T}{2T+1}$. Hence an unbiased estimate of σ_g^2/σ_e^2 will lead to a asymptotically unbiased estimate of h^2.

A diallel cross experiment is said to be complete if each of the $\binom{p}{2}$ crosses appear at least once in the experiment, otherwise it is said to be a partial diallel cross experiment and then necessarily $n < \binom{p}{2}$. Except for a very recent paper of Ghosh and Das (2003), most of the theory of optimal diallel cross designs is based on standard linear model assumptions where the general combining ability effects are taken as fixed and the primary interest lies in comparing the lines with respect to their general combining ability effects. A random effects model has been proposed in Ghosh and Das (2003) that allows one to obtain an estimate of the ratio of the variance components. In order to address the issue of optimal designs they considered the A-optimality criteria for the estimation of heritability in the sense that the designs minimize the sum of the variances of the estimates of the variance components.

In this paper we first propose an unbiased estimate of σ_g^2/σ_e^2 which is a one-to-one function of heritability. We then obtain a large sample expression of the variance of this unbiased estimator of σ_g^2/σ_e^2. Through a simulation study, it is shown that even for small samples, the large sample variance is close to the exact variance. Through minimization of the large sample variance we obtain optimal designs and show certain connections with the optimization problem under the fixed effects model. Some numerical illustrations are given.

2. Unbiased estimates of ratio of variance components and their large sample variances

When a diallel cross experiment with p lines and n crosses is carried out in a completely randomized design (unblocked situation) we can represent our model in matrix notation as

$$Y = \mu 1 + D_1' g + e, \tag{2.1}$$

where Y is the vector of n observations, g is the $p \times 1$ vector of general combining ability effects with $E(g) = 0$ and $D(g) = \sigma_g^2 I$, e is the error vector with $E(e) = 0$ and $D(e) = \sigma_e^2 I$, and $D_1 = (d_{uv}^{(1)})$ is the $p \times n$ line versus observation matrix with $d_{uv}^{(1)} = 1$ if v-th observation is out of a cross involving the u-th line and $d_{uv}^{(1)} = 0$ otherwise. Here 1 represents a column vector of all ones and I denotes an identity matrix. We assume that D_1 has full row rank. Note that,

$$E(Y) = \mu 1_n, D(Y|\sigma_g^2, \sigma_e^2) = \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n. \tag{2.2}$$

As usual, we assume that Y follows a multivariate normal distribution, i.e.,

$$Y \sim N(\mu 1_n, \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n). \tag{2.3}$$

Partitioning the total corrected sum of squares (SST) into the sum of squares due to lines (SSL) and the sum of squares due to error (SSE), based on Henderson's Method III (see Searle, Casella and McCulloch, 1992, page 202), we have $SST = SSL + SSE$ where, $SST = Y'MY$, $SSL = Y'\left[MD_1'\left(D_1MD_1'\right)^{-}D_1M\right]Y$, $SSE = Y'M_0Y$, $M = I - \frac{1}{n}11'$, $M_0 = I - (1\ \ D_1')\left[(1\ \ D_1')'(1\ \ D_1')\right]^{-}(1\ \ D_1')'$ and T^- is a g -inverse of a matrix T .

Let $s = (s_1, s_2, \ldots, s_p)'$ where s_i is the replication of the i -th line. Also, for $i \neq j$, let g_{ij} be the number of times cross (i,j) appears in the design, and $g_{ii} = s_i$. Then it is easy to see that $D_1D_1' = G = (g_{ij})$ and $D_11 = s$. Also, since we assume $Rank(D_1) = p$, G is symmetric with $Rank(G) = p$ and $\mathrm{tr}(G) = 2n$ where for a square matrix A , $\mathrm{tr}(A)$ stands for the trace.

Using the results given in Searle, Casella and McCulloch (1992, pages 204 and 466), the expected values of SSL and SSE reduce to

$$I\!E\begin{bmatrix} SSL \\ SSE \end{bmatrix} = L\begin{pmatrix}\sigma_g^2 \\ \sigma_e^2\end{pmatrix} = L\,\sigma^2, \tag{2.4}$$

where $L = \begin{pmatrix} \mathrm{tr}\left(G - \frac{1}{n}ss'\right) & (p-1) \\ 0 & (n-p) \end{pmatrix}$, and $\sigma^2 = \binom{\sigma_g^2}{\sigma_e^2}$.

Let $C_0 = G - \frac{1}{n}ss'$. Since $C_01 = 0$, $Rank(C_0) \leq p-1$. However, since $Rank(D_1) = p$, it follows that $Rank(C_0) = p-1$. Following Ghosh and Das (2003) the dispersion matrix of $\binom{SSL}{SSE}$ is given by

$$I\!D\begin{pmatrix} SSL \\ SSE \end{pmatrix} = \begin{pmatrix} 2\{\sigma_g^4\,\mathrm{tr}(C_0^2) + 2\sigma_e^2\sigma_g^2\,\mathrm{tr}(C_0) + (p-1)\sigma_e^4\} & 0 \\ 0 & 2(n-p)\,\sigma_e^4 \end{pmatrix}. \tag{2.5}$$

Then the sampling distribution of $\hat{\sigma}^2$ in terms of its sampling variance-covariance matrix follows and is given by

$$I\!D\begin{pmatrix}\hat{\sigma}_g^2 \\ \hat{\sigma}_e^2\end{pmatrix} = L^{-1}I\!D\begin{pmatrix} SSL \\ SSE \end{pmatrix}(L^{-1})' = 2\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \tag{2.6}$$

where $a_{11} = \{(n-p)(\sigma_g^4\,\mathrm{tr}(C_0^2) + 2\sigma_e^2\sigma_g^2\,\mathrm{tr}(C_0) + \sigma_e^4) + \sigma_e^4(p-1)^2\}/\{(n-p)\mathrm{tr}^2(C_0)\}$, $a_{12} = a_{21} = -\sigma_e^4(p-1)/\{(n-p)\,\mathrm{tr}(C_0)\}$ and $a_{22} = \sigma_e^4/(n-p)$.

The following results are well known (e.g., see Searle, Casella and McCulloch, 1992, page 467).

Lemma 2.1 *Let* $Z^{n\times 1} \sim N(\eta, V)$, $\eta \in R^n, V > 0$ *and* A, B *are symmetric non-negative definite matrices of order* n *. Then for given* $\nu = Rank(A)$ *the following hold.*

(a) $Z'AZ \sim \chi_\nu'^2$ *with non-centrality parameter* $\eta' A \eta$ *if and only if* AV *is idempotent.*
(b) $Z'AZ$ *and* $Z'BZ$ *are independently distributed if and only if* $AVB = 0$ *.*
(c) $E(\frac{1}{Z'AZ}) = 1/(\nu - 2)$ *when non-centrality parameter is zero.*

Using the above lemma we have the following result.

Lemma 2.2 *$SSE/\sigma_e^2 \sim \chi^2_{n-p}$ and is distributed independently of SSL .*

For an $n \times n$ real symmetric matrix A , the quadratic form $Y'AY$ is called γ -invariant if $(Y+\gamma 1_n)'A(Y+\gamma 1_n) = Y'AY$ for all real scalars γ . Equivalently, $Y'AY$ is γ -invariant if $A1_n = 0$ or there exists an $n \times n$ symmetric matrix B such that $A = (I - \frac{1}{n}11')B(I - \frac{1}{n}11')$ (see La Motte, 1976). Let H be an $n \times (n-1)$ matrix with i th column $H_i = (i(i+1))^{-\frac{1}{2}}(1_i', -i, 0_{n-i-1}')'$, $i = 1, \ldots, n-1$. The columns of H form an orthonormal basis for the subspace of vectors orthogonal to 1_n and thus $H'H = I_{n-1}$, $HH' = I - 11'/n$. Now if $Y'AY$ is γ -invariant then $Y'AY = Y'HH'BHH'Y = Z'H'BHZ = (HZ)'B(HZ)$ where $Z = H'Y \sim N(0, \sigma_g^2 H'D_1'D_1H + \sigma_e^2 I_{n-1})$.

Following La Motte (1976), let $0 = \lambda_0 < \lambda_1 < \cdots < \lambda_h$ be the $h+1$ distinct eigenvalues of $H'D_1'D_1H$ with multiplicities $m_0, m_1, \ldots, m_h$ respectively. Let $P_i, i = 0, 1, \ldots, h$, be an $(n-1) \times m_i$ matrix whose columns are orthogonal eigenvectors of $H'D_1'D_1H$ corresponding to eigenvalue λ_i . Then the exponent in the density function of Z becomes

$$Z'(\sigma_g^2 H'D_1'D_1H + \sigma_e^2 I)^{-1}Z = \sum_{i=0}^{h}(\sigma_g^2\lambda_i + \sigma_e^2)^{-1}Z'P_iP_i'Z, \tag{2.7}$$

so that $Q_i = Z'P_iP_i'Z,\ i = 0, 1, \ldots, h$ are independent and

$$(\sigma_g^2\lambda_i + \sigma_e^2)^{-1}Q_i, \tag{2.8}$$

follows a central χ^2 -distribution with m_i degrees of freedom, $i = 0, 1, \ldots, h$.

Lemma 2.3 *The quadratic form $Q_i = \sum_{j=1}^{m_i}(w_{ij}'Y)^2, i = 1, \ldots, h$, where $w_{ij} = D_1'\delta$ for some δ , $w_{ij}'w_{i'j'} = 0$, $w_{ij}'1 = 0$, $i, i' = 1, \ldots, h;\ j = 1, \ldots, m_i,\ j' = 1, \ldots, m_{i'}$. Also, the quadratic form $Q_0 = \sum_{j=1}^{m_0}(w_{0j}'Y)^2$ with $w_{0j}'D_1' = 0,\ j = 1, \ldots, m_0$.*

Proof. Observe that $Q_i = Z'P_iP_i'Z = Y'HP_iP_i'H'Y = Y'(HP_i)(HP_i)'Y,\ i = 0, 1, \ldots, h$. Since P_0 is the $(n-1) \times m_0$ matrix of eigen vectors of the matrix $H'D_1'D_1H$ corresponding to the eigenvalue zero , we have $(H'D_1'D_1H)P_0 = 0$ which is equivalent to $(H'D_1')(H'D_1')'P_0 = 0.$ Now since column space of $(H'D_1')(H'D_1')'$ is same as column space of $H'D_1'$, we can equivalently write $D_1HP_0 = 0.$ Hence the second part of the proposition is established. Now using (2.5) we get $(HP_i)'(HP_0) = P_i'H'HP_0 = 0,\ i = 1, \ldots, h$ and $(HP_i)'(HP_j) = P_i'H'HP_j = 0,$ $(HP_i)'1_n = P_i'H'1_n = 0$, $1 \le i < j \le h$. Hence the first assertion of the proposition is established.

Furthermore, $\sum_{i,j,l}(Y_{ijl} - \bar{Y})^2 = Y'HH'Y = Z'Z = Z'(\sum_{i=0}^{k}P_iP_i')Z = \sum_{i=0}^{k}Q_i$, so that Q_i 's partition the total sum of squares into $h+1$ independent quadratics $Q_0, Q_1, \ldots, Q_h$. Here $\bar{Y}$ is the overall mean of $\{Y_{ijl}\}$.

Lemma 2.4 *The non-zero eigenvalues of $H'D_1'D_1H$ are the same as the non-zero eigenvalues of C_0 .*

Under normality of Y , we have the following

Theorem 2.1 *An unbiased estimator of* σ_g^2/σ_e^2 *is* $T = \frac{(n-p-2)(SSL/SSE)-p+1}{tr(C_0)}$.

Proof. From Lemmas 2.1 and 2.2 it follows that $E(SSL/SSE) = E(SSL)E(1/SSE) = \sigma_e^{-2}E(SSL)E(1/(SSE/\sigma_e^2)) = \sigma_e^{-2}E(SSL)E(1/W) = \sigma_e^{-2}E(SSL)/(n-p-2)$ where $W \sim \chi^2_{n-p}$. Now using (2.4) we get $E(SSL/SSE) = \sigma_e^{-2}(\sigma_g^2\mathrm{tr}(C_0) + \sigma_e^2(p-1))/(n-p-2) = ((\sigma_g^2/\sigma_e^2)\mathrm{tr}(C_0) + (p-1))/(n-p-2)$ and the theorem is established.

Theorem 2.2 *Under the assumption that* $\frac{2n}{p} \longrightarrow \omega$ *as* $p \longrightarrow \infty$ *, where* ω *is finite, the large sample variance of* T *is*

$$\alpha_0 \left[p\sigma_g^4 \frac{tr(C_0^2)}{tr^2(C_0)} + 2\sigma_e^2\sigma_g^2 \left(p + (p-1)h_0\right) \frac{1}{tr(C_0)} + (p-1)\sigma_e^4 \left(p+(p-1)h_0\right) \frac{1}{tr^2(C_0)} + \sigma_g^4 h_0 \right], \qquad (2.9)$$

where $\alpha_0 = \frac{2(n-p-2)^2}{p(n-p)^2\sigma_e^4}$ *and* $h_0 = \frac{2(n-p-2)}{(n-p)(\omega-2)}$.

Proof. For some ω , $Var(T) = Var\{\frac{(n-p-2)SSL}{\mathrm{tr}(C_0)SSE}\} = \frac{1}{\omega^2}Var\{\frac{SSL/(\mathrm{tr}(C_0)/\omega)}{SSE/(n-p-2)}\} = \frac{1}{\omega^2}Var\{\frac{SSL^*}{SSE^*}\}$ where $SSL^* = SSL/(\mathrm{tr}(C_0)/\omega)$ and $SSE^* = SSE/(n-p-2)$. Since $\mathrm{tr}(C_0) \le \frac{2n(p-2)}{p}$, under the stated assumption on ω , we have $\frac{\mathrm{tr}(C_0)}{\omega} \simeq 0(p)$. From Lemmas 2.3, 2.4 and equation (2.8) we see that SSL can be expressed as a linear combination of χ^2 random variables, the coefficients being a linear function of the eigenvalues of C_0 (which are bounded quantities). Observing that SSL is a linear combination of independently distributed squared standard normal deviate we have, using Satterthwaite (1946) approximation of linear combination of χ^2 random variables, $Var(SSL^*) = 0\left(\frac{1}{p}\right)$. Now applying Lindberg-Feller central limit theorem we get $p^{1/2}(SSL^* - \theta_1) \xrightarrow{d} N(0, V_1)$ where $\frac{V_1}{p} = Var(SSL^*) = \frac{2\omega^2}{\mathrm{tr}^2(C_0)}\left[\sigma_g^4\mathrm{tr}(C_0^2) + 2\sigma_e^2\sigma_g^2\mathrm{tr}(C_0) + (p-1)\sigma_e^4\right]$ and $\theta_1 = E\left[SSL^*\right] = \frac{\omega}{\mathrm{tr}(C_0)}\left[\sigma_g^2\mathrm{tr}(C_0) + (p-1)\sigma_e^2\right]$.

Similarly, $(n-p-2)^{1/2}(SSE^* - \theta_2) \xrightarrow{d} N(0, V_2)$ which implies $p^{1/2}(SSE^* - \theta_2) \xrightarrow{d} N(0, 2V_2/(\omega-2))$, where $\frac{V_2}{(n-p-2)} = Var(SSE^*) = \frac{2(n-p)\sigma_e^4}{(n-p-2)^2}$ and $\theta_2 = E\left[SSE^*\right] = \frac{n-p}{n-p-2}\sigma_e^2$. Note that from above it follows that $V_2 = \frac{2(n-p)\sigma_e^4}{(n-p-2)}$.

Now, since SSL^* and SSE^* are independently distributed, it follows that $p^{1/2}\begin{pmatrix} SSL^* - \theta_1 \\ SSE^* - \theta_2 \end{pmatrix} \xrightarrow{d} N(0, \Sigma)$ where $\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$ with $\sigma_{11} = V_1$, $\sigma_{22} = \frac{2V_2}{\omega-2} = \frac{4(n-p)}{(\omega-2)(n-p-2)}\sigma_e^4$ and $\sigma_{12} = 0$. Then, by using the central limit theorem on functions of a sequence of multivariate statistics (see Rao (1973), page 387), we get

$$\begin{aligned}
Var(T) &= \frac{1}{p\omega^2}\left[\left(\frac{\partial g(SSL^*, SSE^*)}{\partial SSL^*}\right)^2\Bigg|_{\theta_1,\theta_2} \sigma_{11} + \left(\frac{\partial g(SSL^*, SSE^*)}{\partial SSE^*}\right)^2\Bigg|_{\theta_1,\theta_2} \sigma_{22}\right] \\
&= \frac{2}{p\omega^2}\frac{1}{\theta_2^2}\left[\frac{p\omega^2}{\mathrm{tr}^2(C_0)}\left\{\sigma_g^4\mathrm{tr}(C_0^2) + 2\sigma_e^2\sigma_g^2\mathrm{tr}(C_0) + (p-1)\sigma_e^4\right\}\right. \\
&\quad \left. + \frac{2\omega^2}{\mathrm{tr}^2(C_0)}(\sigma_g^2\mathrm{tr}(C_0) + (p-1)\sigma_e^2)^2 \frac{(n-p-2)}{(n-p)(\omega-2)}\right] \\
&= \frac{2}{p}\frac{(n-p-2)^2}{(n-p)^2}\frac{1}{\sigma_e^4}\left[\frac{\mathrm{tr}(C_0^2)}{\mathrm{tr}^2(C_0)}p\sigma_g^4 + \frac{1}{\mathrm{tr}(C_0)}\left\{2\sigma_e^2\sigma_g^2 p + 4\sigma_e^2\sigma_g^2(p-1)\frac{n-p-2}{(n-p)(\omega-2)}\right\}\right.
\end{aligned}$$

$$+\frac{1}{\mathrm{tr}^2(C_0)}\left\{p(p-1)\sigma_e^4+2(p-1)^2\sigma_e^4\frac{n-p-2}{(n-p)(\omega-2)}\right\}+\frac{2(n-p-2)}{(n-p)(\omega-2)}\sigma_g^4\Bigg].$$

$$= \frac{2}{p}\frac{(n-p-2)^2}{(n-p)^2}\frac{1}{\sigma_e^4}\left[p\sigma_g^4\frac{\mathrm{tr}(C_0^2)}{\mathrm{tr}^2(C_0)}+2\sigma_e^2\sigma_g^2\left(p+\frac{2(p-1)(n-p-2)}{(\omega-2)(n-p)}\right)\frac{1}{\mathrm{tr}(C_0)}\right.$$

$$\left.+(p-1)\sigma_e^4\left(p+\frac{2(p-1)(n-p-2)}{(n-p)(\omega-2)}\right)\frac{1}{\mathrm{tr}^2(C_0)}+\frac{2(n-p-2)}{(n-p)(\omega-2)}\sigma_g^4\right].$$

This completes the proof.

Now consider a diallel cross experiment carried out using a block design involving p lines and b blocks each having k crosses ($n = bk$). Here our model is

$$Y = \mu 1 + D_2'\beta + D_1'g + e, \tag{2.10}$$

where as before, Y is the vector of n observations, g is the $p\times 1$ vector of general combining ability effects with $\mathbb{E}(g) = 0$ and $\mathbb{D}(g) = \sigma_g^2 I$, β is the fixed effect due to blocks and e is the error vector with $\mathbb{E}(e) = 0$ and $\mathbb{D}(e) = \sigma_e^2 I$. Also, $D_1 = (d_{uv}^{(1)})$ is as mentioned earlier, and $D_2 = (d_{uv}^{(2)})$ is the $b \times n$ block versus observation matrix with $d_{uv}^{(2)} = 1$ if the v -th observation arise from the u -th block and $d_{uv}^{(2)} = 0$ otherwise. Thus, $\mathbb{E}(Y) = \mu 1_n, \mathbb{D}(Y|\sigma_g^2, \sigma_e^2) = \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n$. Again, we assume that $Y \sim N(\mu 1_n, \sigma_g^2 D_1' D_1 + \sigma_e^2 I_n)$. Let $N = (n_{ij})$ with n_{ij} indicating the number of times the i -th line occurs in the j -th block, and $C = G - k^{-1}NN'$. Note that since $C1 = 0$, $Rank(C) \le p-1$. Here $Rank(C) = p-1$ since we assume that $D_2'1 = \frac{1}{2}D_1'1 = 1$ are the only two independent restrictions among the columns of the design matrix.

Now, as in the case of unblocked model, we obtain, after routine algebra, the expected values of SSL and SSE which are given by

$$\mathbb{E}\begin{bmatrix} SSL \\ SSE \end{bmatrix} = L\begin{pmatrix}\sigma_g^2 \\ \sigma_e^2\end{pmatrix} = L\,\sigma^2, \tag{2.11}$$

where $L = \begin{pmatrix} \mathrm{tr}(C) & p-1 \\ 0 & n-b-p+1 \end{pmatrix}$.

Also,

$$\mathbb{D}\begin{pmatrix} SSL \\ SSE \end{pmatrix} = \begin{pmatrix} 2\{\sigma_g^4\ \mathrm{tr}(C^2) + 2\sigma_e^2\sigma_g^2\ \mathrm{tr}(C) + \sigma_e^4\ (p-1)\} & 0 \\ 0 & 2(n-b-p+1)\ \sigma_e^4 \end{pmatrix}. \tag{2.12}$$

and

$$\mathbb{D}\begin{pmatrix}\hat\sigma_g^2 \\ \hat\sigma_e^2\end{pmatrix} = L^{-1}\mathbb{D}\begin{pmatrix} SSL \\ SSE \end{pmatrix}(L^{-1})' = 2\begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22}\end{pmatrix}, \tag{2.13}$$

where

$t_{11} = \{(n-b-p+1)(\sigma_g^4\ \mathrm{tr}(C^2) + 2\sigma_e^2\sigma_g^2\ \mathrm{tr}(C) + \sigma_e^4) + \sigma_e^4\ (p-1)^2\}/\{(n-b-p+1)\ \mathrm{tr}^2(C)\}$,

$t_{12} = t_{21} = -\sigma_e^4\ (p-1)/\{(n-b-p+1)\ \mathrm{tr}(C)\}$,

and

$t_{22} = \sigma_e^4/(n-b-p+1)$.

Let H^* be an $n \times (n-b)$ matrix such that

$$H^{*\prime}H^* = I_{n-b}, \qquad H^*H^{*\prime} = I - (1\ \ D_2')[(1\ \ D_2')'(1\ \ D_2')]^-(1\ \ D_2')'. \tag{2.14}$$

Note that $D_2H^* = 0$ and $1_n'H^* = 0$.

Then, $Z_B^{(n-b)\times 1} = H^{*\prime}Y \sim N(0, \sigma_g^2 H^{*\prime}D_1'D_1H^* + \sigma_e^2 I_{n-b})$

As in the previous section, let $0 = \lambda_0 < \lambda_1 < \cdots < \lambda_h$ be the $h+1$ distinct eigen values of $H^{*'}D_1'D_1H^*$, with multiplicities $m_0, m_1, \ldots, m_h$ respectively. Let P_{B_i}, $i = 0, \ldots, h$ be an $(n-b)\times m_i$ matrix whose columns are orthogonal eigen vectors of $H^{*'}D_1'D_1H^*$ corresponding to λ_i. Then the exponent in the density function of Z_B becomes

$$Z_B'(\sigma_g^2 H^{*'}D_1'D_1H^* + \sigma_e^2 I)^{-1}Z_B = \sum_{i=0}^{h}(\sigma_g^2\lambda_i + \sigma_e^2)^{-1}Z_B'P_{B_i}P_{B_i}'Z_B, \tag{2.15}$$

so that $Q_{B_i} = Z_B'P_{B_i}P_{B_i}'Z_B$, $i = 0, \ldots, h$ are independent and

$$(\sigma_g^2\lambda_i + \sigma_e^2)^{-1}Q_{B_i} \tag{2.16}$$

follows a central χ^2 distribution with m_i degrees of freedom, $i = 0, \ldots, h$.

Lemma 2.5 *The quadratic forms $Q_{B_i}, i = 1, \ldots, h$ are generated from the sum of squares of linear combinations of Y, i.e., $Q_{B_i} = \sum_{j=1}^{m_i}(w_{ij}'Y)^2$ where $w_{ij} = D_1^{*'}\delta$ for some δ, $D_1^*D_2' = 0$, $w_{ij}'w_{i'j'} = 0$, $i, i' = 1, \ldots, h;\ j = 1, \ldots, m_i,\ j' = 1, \ldots m_{i'}$. Also, the quadratic form $Q_{B_0} = \sum_{j=1}^{m_0}(w_{0j}'Y)^2$ represents the sum of squares generated with $w_{0j}'(D_1'\ \ D_2') = 0,\ j = 1, \ldots, m_0$.*

Lemma 2.6 *The non-zero eigenvalues of $H^{*'}D_1'D_1H^*$ is the same as the non-zero eigenvalues of C.*

Under normality of Y, we have the following results whose proof follows on lines similar to the proofs of Theorems 2.1 and 2.2.

Theorem 2.3 *An unbiased estimator of σ_g^2/σ_e^2 is $T = \frac{(n-b-p-1)(SSL/SSE)-p+1}{tr(C)}$.*

Theorem 2.4 *Under the assumption that $\frac{2n}{p} \longrightarrow \omega_1$ as $p \longrightarrow \infty$, where ω_1 is finite, the large sample variance of T is*

$$\alpha_1\left[p\sigma_g^4\frac{tr(C^2)}{tr^2(C)} + 2\sigma_e^2\sigma_g^2\left(p + (p-1)h_1\right)\frac{1}{tr(C)} + (p-1)\sigma_e^4\left(p + (p-1)h_1\right)\frac{1}{tr^2(C)} + \sigma_g^4 h_1\right], \tag{2.17}$$

where $\alpha_1 = \frac{2(n-b-p-1)^2}{p(n-b-p+1)^2\sigma_e^4}$ and $h_1 = \frac{2(n-b-p-1)}{(n-b-p+1)(\omega_1-2)}$.

3. Optimal designs and a simulation study

Let $\mathcal{D}(p,n)$ be the class of unblocked designs for diallel crosses involving p lines and n crosses and $\mathcal{D}(p,b,k)$ the class of diallel cross designs with p lines arranged in b blocks of k crosses each. Also, we use $\mathcal{D}_0(p,n)$ to denote the subclass of designs in $\mathcal{D}(p,n)$ having designs with $s_i = s = 2n/p\,; i = 1, \ldots, p$. In fact, among designs in $\mathcal{D}(p,n)$, only designs in the subclass $\mathcal{D}_0(p,n)$ have maximal $\mathrm{tr}(C_0)$. Finally, let $\mathcal{D}_0(p,b,k)$ be the subclass of designs in $\mathcal{D}(p,b,k)$ for which $\mathrm{tr}(C)$ is maximum. A design d is said to be optimal if, among all designs in $\mathcal{D}$, d minimizes the large sample variance of T.

In the unblocked situation, in order to minimize the large sample variance of T as given in (2.9), within the class of designs $\mathcal{D}(p,n)$, it is sufficient to minimize $\frac{\text{tr}(C_0^2)}{\text{tr}^2(C_0)}$ and $\frac{1}{\text{tr}(C_0)}$. Similarly from (2.17) it follows that an optimal design in $\mathcal{D}(p,b,k)$ minimizes $\frac{\text{tr}(C^2)}{\text{tr}^2(C)}$ and $\frac{1}{\text{tr}(C)}$. In other words, from (2.9) and (2.17) we observe that the minimization problem addressed in Ghosh and Das (2003) is analogus to the minimization of large sample variance of T. Thus, A-optimal designs obtained in Ghosh and Das(2003) are also optimal for the minimization of the large sample variance of the unbiased estimator of the ratio of variance components σ_g^2/σ_e^2.

Henceforth, by optimal we mean optimal in the sense of minimization of large sample variance, $Var(T)$, of T. Making an appeal to the results of Ghosh and Das (2003), we have the following results.

Theorem 3.1 *Let $d_0^* \in \mathcal{D}(p,n)$ be a design for diallel crosses, and suppose $C_{0d_0^*}$ satisfies (i) tr $(C_{0d_0^*}) = 2n(p-1)/p$, and (ii) $C_{0d_0^*}$ is completely symmetric in the sense that $C_{0d_0^*}$ has all its diagonal elements equal and all its off-diagonal elements equal. Then d_0^* is optimal in $\mathcal{D}(p,n)$.*

Theorem 3.2 *Let $d^* \in \mathcal{D}(p,b,k)$ be a block design for diallel crosses with $x = [2k/p]$ ($[z]$ denoting the largest integer not exceeding z) and suppose C_{d^*} satisfies (i) tr $(C_{d^*}) = k^{-1}b\{2k(k-1-2x)+px(x+1)\}$, and (ii) C_{d^*} is completely symmetric. Then d^* is optimal in $\mathcal{D}(p,b,k)$.*

Theorem 3.1 establishes the optimality of complete diallel cross designs in $\mathcal{D}(p,n)$. Theorem 3.2 implies that the existence of a nested balanced incomplete block design d with parameters $v = p, b_1 = b, b_2 = bk, k_1 = 2k, k_2 = 2$ would yield an optimal incomplete block design d^* for diallel crosses. The construction methods and elaborate tables of nested balanced incomplete block designs are available in a recent review paper by Morgan, Preece and Rees (2001). The tables in their paper provide solutions to our optimal diallel cross designs within the parametric range $2k < p < 16,\ s \leq 30$. The case $2k = p$ is dealt in Gupta and Kageyama (1994). The nested balanced incomplete block designs have been extended to nested balanced block designs and a series of designs, optimal under our setup, is given in Das, Dey and Dean (1998).

Two theorems follow.

Theorem 3.3 *A design d_0^* with p lines is optimal in $\mathcal{D}_0(p,n)$ with $s = 2n/p$ if and only if the number of times, $g_{d_0^*ii'}$, that cross (i,i') occurs in d_0^* satisfies $|g_{d_0^*ii'} - s/(p-1)| < 1$ for $i \neq i',\ i,i' = 1,\ldots,p.$*

Theorem 3.4 *A design d^* in $\mathcal{D}_0(p,b,k)$ with $2k/p$ an integer is optimal in $\mathcal{D}_0(p,b,k)$ if and only if the number of times, $g_{d^*ii'}$, that cross (i,i') occurs in d^* satisfies $|g_{d^*ii'} - s/(p-1)| < 1$ for $i \neq i',\ i,i' = 1,\ldots,p.$*

From Theorem 3.3, partial diallel cross designs in which every line appears the same number $s = 2n/p$ of times and in which each cross appears either $\lambda = [s/(p-1)]$ or $\lambda + 1$ times are optimal. A common way to construct a partial diallel cross design is to form crosses between the two treatments in each block of a conventional binary incomplete block design with p treatments each occurring s times, n distinct blocks of size 2 each and treatment concurrences λ and $\lambda + 1$. Any such partial diallel cross design satisfies the conditions of Theorem 3.3 and is optimal. Among others, this includes the M-designs of Singh and Hinkelmann (1995), the first series of designs of Mukerjee (1997), and some other designs as listed in Das, Dean and Gupta (1998).

Das, Dean and Gupta (1998) gave two general methods of construction of block designs for partial diallel crosses. Their designs belong to $\mathcal{D}_0(p,b,k)$ with $2k/p$ an integer. Moreover the designs satisfy the conditions of Theorem 3.4 and are thus optimal in $\mathcal{D}_0(p,b,k)$.

As a result of the very nature of the derived objective function under the model, that we are minimizing, every previously known MS-optimal design under the fixed effects model would be optimal under our set-up.

Now through a simulation study, we show that even for small samples, the large sample variance is close to the exact variance. The study of optimal designs for the estimation of the ratio of variance components from its large sample variance expression has been justified by the exhaustive simulation of the observations from normal population with its covariance structure depending upon the design matrices D_1, D_2 and the variance components σ_g^2 and σ_e^2. We show that even for small samples, the large sample variance is close to the exact variance. Two optimal designs d_1 and d_2 have been taken from the class of unblocked diallel cross designs, the classes being $\mathcal{D}(5,10)$ and $\mathcal{D}_0(8,16)$ respectively and one optimal design d_3 from the class $\mathcal{D}(7,7,3)$ of blocked diallel cross designs. In case of $\mathcal{D}(5,10)$ the optimal design for estimating the ratio of variance components σ_g^2/σ_e^2 in the class of unblocked diallel cross design with 10 observation and 5 inbred lines is found where each of the 10 crosses has appeared exactly once in the design. The estimator has been computed based on the observation vector of dimension 10 which follows a multivariate normal distribution will covariance matrix $\sigma_g^2 D_1' D_1 + \sigma_e^2 I_{10}$ and mean vector $\mu 1_{10}$, in each of the iteration. The variance of the iterated values of the estimator is then computed and compared with numerical value of the corresponding large sample variance, as shown below in Table-1. Throughout we have obtained the exact variance by using (i) SAS Random Number technique and (ii) Box Muller transformation. In the tables the column under ($*$) corresponds to variances obtained by Box-Muller transformation. Similar simulation technique has been carried out (presented in Tables 2 and 3) for optimal designs in $\mathcal{D}_0(8,16)$ and $\mathcal{D}(7,7,3)$. The number of iterations in the simulation ranges from 30, 35, 40, 45, 50. It is to be noted that for d_1 and d_3, the large sample variance is quite close to the variance from the estimates simulated in the iterative procedure although $w = w_1 = \frac{2n}{p} = p - 1$.

Table-1: Complete diallel cross with 5 lines in $\mathcal{D}(5,10)$. (1) stands for $\sigma_g^2 = \sigma_e^2 = 1$ with large sample variance

0.473. (2) stands for $\sigma_g^2 = 1.5$, $\sigma_e^2 = 1$ with large sample variance 0.898.

Number of Iteration	(1)	(2)	(1*)	(2*)
30	0.386	0.759	0.412	0.717
35	0.392	0.785	0.412	0.747
40	0.429	0.811	0.427	0.752
45	0.457	0.812	0.460	0.769
50	0.488	0.857	0.494	0.859

Table-2: Optimal partial diallel cross design with 8 lines in $\mathcal{D}_0(8,16)$. (1) stands for $\sigma_g^2 = \sigma_e^2 = 1$, with large sample variance 0.652. (2) stands for $\sigma_g^2 = 1.5$, $\sigma_e^2 = 1$ with large sample variance 0.306.

Number of Iteration	(1)	(2)	(1*)	(2*)
30	0.617	0.337	0.645	0.316
35	0.617	0.346	0.654	0.315
40	0.622	0.356	0.654	0.327
45	0.622	0.357	0.635	0.328
50	0.642	0.357	0.653	0.336

Table-3: Complete blocked diallel cross with 7 lines, 7 Blocks, Blocks size 3 in $\mathcal{D}(7,7,3)$. (1) stands for $\sigma_g^2 = \sigma_e^2 = 1.0$ with large sample variance 0.366. (2) stands for $\sigma_g^2 = 1.5$, $\sigma_e^2 = 1$ with large sample variance 0.793.

Number of Iteration	(1)	(2)	(1*)	(2*)
30	0.317	0.740	0.324	0.747
35	0.323	0.740	0.321	0.744
40	0.322	0.738	0.321	0.754
45	0.323	0.754	0.346	0.768
50	0.321	0.788	0.344	0.785

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