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ON OPTIMAL ROW-COLUMN DESIGNS FOR TWO TREATMENTS

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On optimal row-column designs for two treatments

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Abstract: This paper presents optimal 3×3, 3×4, and 3×5 row-column designs for two treatments in the presence of a symmetric doubly geometric correlated errors. All designs presented here minimize the variance of generalized least squares estimator of the difference between treatment effects under a correlated model that incorporates both fixed row and fixed column effects.

1. Introduction

An allocation of of $v \geq 2$ treatments to pq experimental units, which are further grouped into p rows and q columns, is called a row-column design. This paper addresses the problem of choosing a row-column design d that estimates the difference between the effects of two treatments with minimum variance under the model

$$Y_d = 1_{pq}\mu + Z_1\rho + Z_2\gamma + X_d\tau + \epsilon, \quad \text{cov}(\epsilon) = V. \tag{1.1}$$

Here Y_d (written in column order) is the $pq \times 1$ response vector, 1_n is the $n \times 1$ column vector of ones, τ is the $v \times 1$ vector of treatment effects, X_d is a $pq \times v$ plot-treatment design matrix that defines the allocation of treatments to the experimental units according to the design d, and ρ and γ are vectors of parameters for fixed row and fixed column effects, respectively. The matrices $Z_1 = 1_q \otimes I_p$ and $Z_2 = I_q \otimes 1_p$ are called the plot-row and plot-column incidence matrices, respectively. The error co-variance matrix is assumed here to be a special case ($\alpha = \beta$) of the following doubly geometric process :

$$V = \frac{\sigma^2(1-\alpha^2)^{-1}}{(1-\beta^2)} \begin{pmatrix} 1 & \beta & \beta^2 & \dots & \beta^{q-1} \\ \beta & 1 & \beta & \dots & \beta^{q-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \beta^{q-1} & \beta^{q-2} & \beta^{q-3} & \dots & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \alpha & \alpha^2 & \dots & \alpha^{p-1} \\ \alpha & 1 & \alpha & \dots & \alpha^{p-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha^{p-1} & \alpha^{p-2} & \alpha^{p-3} & \dots & 1 \end{pmatrix}.$$

With $Z = (1_{pq} \;\; Z_2 \;\; Z_1)$, the generalized least squares information matrix C_d for estimation of treatment contrasts under (1.1) can be written as

$$C_d = X_d' V^{-1} X_d - X_d' V^{-1} Z (Z' V^{-1} Z)^{-} Z' V^{-1} X_d. \tag{1.2}$$

The matrix C_d, for any connected design d, is nonnegative definite with rank $v-1$. For $v=2$, C_d is of order 2×2 and of the following form

$$C_d = \begin{pmatrix} c_{d11} & -c_{d11} \\ -c_{d11} & c_{d11} \end{pmatrix}$$

where c_{d11} must be determined by simplifying the matrix C_d given by (1.2). This simplified form of C_d implies that the $\text{var}_d(\hat{\tau}_1 - \hat{\tau}_2) = c_{d11}^{-1}$ for a design d. If we let $D(2,p,q)$ denote the class of all connected $p \times q$ row-column designs for two treatments, then a design $d^* \in D(2,p,q)$ is optimal if $\text{var}_{d^*}(\hat{\tau}_1 - \hat{\tau}_2) = c_{d^*11}^{-1} \leq c_{d11}^{-1} = \text{var}_d(\hat{\tau}_1 - \hat{\tau}_2)$ for all $d \in D(2,p,q)$. This is equivalent to saying that the design d^* is optimal if $c_{d^*11} \geq c_{d11}$ for all $d \in D(2,p,q)$.

Several researchers have addressed the problems of optimality of row-column designs for $v \geq 2$ when observations are correlated (e.g., Gill and Shukla, 1985; Kunert, 1988; Martin, 1986; Martin and Eccleston, 1993; Morgan and Uddin, 1991, 1998; Uddin and Morgan, 1991, 1997a, 1997b; Uddin, 1997). Optimal $p \times q$ row-column designs under the model (1.1), that incorporates both row and column effects, are almost nonexistent except for some very special cases. Uddin and Morgan (1997a) have attempted to determine universally optimal two-dimensional block designs for correlated observations with and without row/column effects in (1.1). Their paper gives some universally optimal $p \times 2$ row-column designs under (1.1) when $v = 2$. For $v \geq 3$, their universally optimal designs use $b \geq 2$ blocks each of which is a $p \times 2$ row-column design. For $v = 2$, Uddin (1997) gives universally optimal $p \times q$ designs for all even p and q when both α and β are positive. More specifically, it is shown in Uddin (1997) that the design

$$d^* = \begin{pmatrix} 1 & 2 & 1 & 2 & \dots & 1 & 2 \\ 2 & 1 & 2 & 1 & \dots & 2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 2 & 1 & 2 & \dots & 1 & 2 \\ 2 & 1 & 2 & 1 & \dots & 2 & 1 \end{pmatrix}_{p \times q}$$

is universally optimal (in the sense of Kiefer, 1975) over $D(v = 2, p, q)$ for all $\alpha \geq 0$, $\beta \geq 0$ and for all even p and q. The author is not aware of any other paper that gives optimal designs in the present set-up. It appears that even for the special case of $v = 2$, the optimality problem is only partially solved under the model (1.1). For example, optimal $p \times q$ designs are not known for all $\alpha, \beta \in (-1, 1)$ when at least one of $p \geq 3$ and $q \geq 3$ is odd. At this time, we do not know if optimal $p \times q$ designs for two treatments can be determined for all p, q, α and β mentioned above ; see the information matrix C_d in Uddin (1997) and the algebraic complexity involved in the determination of such optimal designs. However, for small p and q, the problem can be solved by enumerating all possible designs for a given p and q. In this paper, we have determined optimal 3×3, 3×4, and 3×5 designs for two treatments under (1.1) with $\alpha = \beta$. We have enumerated all possible designs in each case and determined optimal designs by comparing c_{d11} of all designs for a given p and q. Our results are presented in the following section.

2. Optimal designs for $v = 2$.

We have utilized MAPLE software to simplify the information matrix C_d and obtained c_{d11} for all possible $d \in D(v = 2, p, q)$ for each combination of p and q mentioned above. Note that two treatments can be assigned to pq experimental units in 2^{pq} ways, each of these arrangement is a $p \times q$ design. However, not all of these designs are connected since C_d is a zero matrix for some d. In our search of optimal designs, we have calculated c_{d11} element of C_d for each connected design d. The optimal design is one that maximizes c_{d11} over $D(v = 2, p, q)$ for $\alpha \in (-1, 1)$. However, no single design is found that maximizes c_{d11} over $D(2, p, q)$ for all $\alpha \in (-1, 1)$. The optimal design depends on the magnitude of p , q and α.

In the following subsections, we use the convention that two designs d_1 and d_2 are distinct if d_1 can not be obtained from d_2 by interchanging the two symbols 1 and 2 in d_2, or d_1 can not be obtained by rotating the design d_2.

2.1 Optimal 3×3 designs for $v = 2$.

In this case, c_{d11} of all connected 3×3 designs are obtained using MAPLE software. We have found four distinct designs d_1, d_1', d_2, and d_3 such that the $\max(c_{d_1 11}, c_{d_1' 11}, c_{d_2 11}, c_{d_3 11})$, for each $\alpha \in (-1, 1)$, is greater than or equal to the c_{d11} values of all other 3×3 designs. Thus the c_{d11} values of these four designs may be compared to determine optimal designs.

For the purpose of determining the values of α and the corresponding optimal designs, we first list in Table 1 these four distinct designs and the c_{d11} element of the corresponding C_d.

Table 1. Four distinct designs and the corresponding c_{d11}

Design	c_{d11}
$d_1 = \begin{pmatrix} 2 & 2 & 1 \\ 2 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$	$\frac{-16\alpha^4+32\alpha^3-32\alpha+16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}$
$d_1' = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 2 \\ 2 & 2 & 1 \end{pmatrix}$	$\frac{-16\alpha^4+32\alpha^3-32\alpha+16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}$
$d_2 = \begin{pmatrix} 2 & 2 & 1 \\ 2 & 1 & 2 \\ 1 & 2 & 2 \end{pmatrix}$	$\frac{-10\alpha^6+8\alpha^5+6\alpha^4+16\alpha^3-14\alpha^2-24\alpha+18}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}$
$d_3 = \begin{pmatrix} 2 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix}$	$\frac{-16\alpha^6+48\alpha^4-48\alpha^2+16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}$

Note that the two distinct designs d_1 and d_1' have the same c_{d11}. Utilizing MAPLE, we have compared c_{d11} values of all 3×3 designs. It follows that $\max_{\alpha \in (-1,1)}(c_{d_1 11} = c_{d_1' 11},\ c_{d_2 11},\ c_{d_3 11})$ $\geq c_{d11}$, for all other $d \in D(2, 3, 3)$. Hence the values of α and the corresponding optimal design can be determined by comparing c_{d11} of the above four designs. The values of α for which $c_{d_1 11}$ or $c_{d_1' 11}$ is greater than $c_{d_2 11}$ and $c_{d_3 11}$ are determined by solving the inequalities

$$\frac{-16\alpha^4 + 32\alpha^3 - 32\alpha + 16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)} > \frac{-10\alpha^6 + 8\alpha^5 + 6\alpha^4 + 16\alpha^3 - 14\alpha^2 - 24\alpha + 18}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}$$

and

$$\frac{-16\alpha^4 + 32\alpha^3 - 32\alpha + 16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)} > \frac{-16\alpha^6 + 48\alpha^4 - 48\alpha^2 + 16}{(3-\alpha)^2(1-\alpha)^2(1-\alpha^2)}.$$

The above two inequalities are satisfied for all $\alpha \in (-1, -1/5)$. Hence d_1 and d'_1 are optimal under (1.1) for all $\alpha \in (-1, -1/5)$. In a similar fashion, are obtained the values of α for which d_2 and d_3 are optimal. These values of α and the corresponding optimal (maximal c_{d11}) designs are reported in Table 2 below.

Table 2 . Optimal 3×3 designs

α	Optimal design
$(-1, \frac{-1}{5})$	$d_1 = \begin{pmatrix} 2 & 2 & 1 \\ 2 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$, $d'_1 == \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 2 \\ 2 & 2 & 1 \end{pmatrix}$
$(\frac{-1}{5}, \frac{2\sqrt{7}-5}{3})$	$d_2 = \begin{pmatrix} 2 & 2 & 1 \\ 2 & 1 & 2 \\ 1 & 2 & 2 \end{pmatrix}$
$(\frac{2\sqrt{7}-5}{3}, 1))$	$d_3 = \begin{pmatrix} 2 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix}$

2.2. Optimal 3×4 designs

Optimal 3×4 designs are obtained by comparing c_{d11} of all possible 3×4 designs. In this case, we have found two designs that maximize, depending on α, the c_{d11} element of the information matrix C_d. The values of α and the corresponding optimal 3×4 designs are in Table 2.

Table 2. Optimal 3×4 designs

α	Optimal design
$(-1, 0)$	$d_4 = \begin{pmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ 2 & 2 & 1 & 1 \end{pmatrix}$
$(0, 1)$	$d_5 = \begin{pmatrix} 1 & 2 & 1 & 2 \\ 2 & 1 & 2 & 1 \\ 1 & 2 & 1 & 2 \end{pmatrix}$

The c_{d11} for designs d_4 and d_5 are as follows.

$$c_{d_4 11} = \frac{-8\alpha^{10} + 64\alpha^8 - 176\alpha^6 + 224\alpha^4 - 136\alpha^2 + 32}{(3-\alpha)(1-\alpha)^2(1-\alpha^2)^2(4-2\alpha)}$$

$$c_{d_5 11} = \frac{-8\alpha^9 + 40\alpha^8 - 72\alpha^7 + 40\alpha^6 + 72\alpha^5 - 168\alpha^4 + 104\alpha^3 + 56\alpha^2 - 96\alpha + 32}{(3-\alpha)(1-\alpha)^2(1-\alpha^2)^2(4-2\alpha)}.$$

The values of α in Table 2 above are determined by solving the inequality $c_{d_4 11} > c_{d_5 11}$.

2.3 Optimal 3×5 designs.

The procedure used for the determination of optimal 3×5 designs is similar to that of 3×3 and 3×4 designs. Optimal 3×5 designs are obtained by comparing c_{d11} of all 3×5 designs. The distinct designs that are found to be optimal are reported in Table 3.

Table 3. Optimal 3×5 designs

α	Optimal Designs	c_{d11}
$(-1, -0.05561673968]$	$\{\begin{pmatrix} 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 2 & 1 & 1 \\ 2 & 2 & 1 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 1 & 1 & 1 \\ 2 & 2 & 1 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 1 & 2 & 2 \\ 2 & 2 & 2 & 1 & 1 \\ 2 & 2 & 2 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 1 & 2 & 2 \\ 2 & 2 & 1 & 1 & 1 \\ 2 & 2 & 2 & 1 & 1 \end{pmatrix}\}$	$\frac{48-160\alpha+176\alpha^2-16\alpha^3-144\alpha^4+160\alpha^5-80\alpha^6+16\alpha^7}{(3-\alpha)(5-3\alpha)(1-\alpha)^2(1-\alpha^2)}$
$[-0.05561673969, 0)$	$\begin{pmatrix} 1 & 1 & 2 & 2 & 1 \\ 2 & 2 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 & 2 \end{pmatrix}$	$\frac{50-130\alpha+74\alpha^2+78\alpha^3-130\alpha^4+74\alpha^5-2\alpha^6-22\alpha^7+8\alpha^8}{(3-\alpha)(5-3\alpha)(1-\alpha)^2(1-\alpha^2)}$
$(0, 0.05414365096]$	$\begin{pmatrix} 1 & 2 & 1 & 2 & 1 \\ 2 & 1 & 2 & 1 & 1 \\ 1 & 2 & 1 & 1 & 2 \end{pmatrix}$	$\frac{50-40\alpha-106\alpha^2+52\alpha^3+98\alpha^4-8\alpha^5-54\alpha^6-4\alpha^7+12\alpha^8}{(3-\alpha)(5-3\alpha)(1-\alpha)^2(1-\alpha^2)}$
$[0.05414365097, 1)$	$\begin{pmatrix} 1 & 2 & 1 & 2 & 1 \\ 2 & 1 & 2 & 1 & 2 \\ 1 & 2 & 1 & 2 & 1 \end{pmatrix}$	$\frac{48-160\alpha^2+192\alpha^4-96\alpha^6+16\alpha^8}{(3-\alpha)(5-3\alpha)(1-\alpha)^2(1-\alpha^2)}$

The first four designs in Table 3 above have the same c_{d11} and hence are equally good. The values of α in column one are determined by comparing the c_{d11} values reported in third column under c_{d11}.

Note that the optimal $p \times q$ design (with $p \leq q$) for two treatments, when $\alpha = 0$ (errors are uncorrelated) and both p and q are odd, uses treatment one $p(q-1)/2$ times and treatment two $p(q+1)/2$ times, see Morgan and Uddin (1993). Thus the optimal designs with uncorrelated errors require that the two treatment replications differ by p. However, this is not the case for our optimal designs with large $|\alpha|$, see the designs in Tables 1 and 3 for large $|\alpha|$. Here the difference between the replications of two treatments is one, a criterion often preferred by practicing statisticians.

We have determined only 3×3, 3×4 and 3×5 optimal row-column designs for two treatments. It would be unwise to make any recommendation for all $p \times q$ designs based on these three designs. However, we suspect that the treatment allocation patterns found here, if extended to $p \times q$ designs, will give optimal $p \times q$ designs especially for large $|\alpha|$. For example, a design in which no treatment is neighbored by itself in rows and in columns is expected to be optimal for large positive α.

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