Journal of Statistical Planning and Inference 19 (1988) 261-267
North-Holland

NON-EQUIREPLICATE KRONECKER FACTORIAL DESIGNS

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Received 31 December 1986; revised manuscript received 8 June 1987
Recommended by D. Raghavarao

Abstract: Considering non-equireplicate factorial designs based on the Kronecker product of varietal designs, it is seen that the factorial effect efficiencies in such designs can be controlled by suitably choosing the initial varietal designs.

AMS Subject Classification: 62K15.

Key words and phrases: Efficiency; Kronecker product; unequal replication.

1. Introduction

In recent years two broad methods emerged for the construction of factorial designs: (a) factorial experiments in generalized cyclic designs (John (1973a,b), Dean and John (1975), Dean and Lewis (1980); for a comprehensive list of references see John and Lewis (1983)) and (b) use of Kronecker or Kronecker-type products (Mukerjee (1981, 1986), Gupta (1983, 1985, 1986), Mukerjee and Sen (1988)). Both these methods lead to designs with orthogonal factorial structure (OFS) and, if used appropriately, are capable of ensuring high efficiencies on the factorial effects of interest.

It, however, appears that these methods have so far been applied only for the construction of equireplicate designs. The same remark also holds good for most of the classical procedures (see e.g., Voss (1986)). In general, non-equireplicate factorial designs have apparently received rather little attention in the literature although some work has been reported among others by Puri and Nigam (1978). One reason may be that with unequal numbers of replications it is hard to retain OFS and consequently, an investigation on the factorial effect efficiencies as also the analysis of the design itself, may become difficult. On the other hand, non-equireplicate designs are of much practical importance simply because in most practical situations the treatment combinations in a factorial experiment are not all equally expensive. In

0378-3758/88/$3.50

such situations, the use of equireplicate designs may become either too expensive or wasteful.

In an attempt to fill up this gap to some extent, the present paper extends the method (b) above to generate non-equireplicate factorial designs. The designs so constructed may not have OFS, but most of the advantages ensuing from OFS are retained. Thus (i) one can ensure high interaction efficiencies in the resulting factorial designs by suitably choosing the initial varietal designs and (ii) the analysis of the factorial designs obtained by the method is fairly simple. Sections 3 and 4 deal with the aspects (i) and (ii) respectively.

2. Notation and preliminaries

Throughout the paper, whether the design under consideration is varietal or factorial, the fixed effects intrablock model, with independent homoscedastic errors and no block-treatment interaction, is assumed. Let for $1 \le j \le m$, D_j be a varietal design involving s_j varieties and having an $s_j \times b_j$ incidence matrix N_j. Let $r_{j0}, r_{j1}, \ldots, r_{js_j-1}$ be the replication numbers and $k_{j0}, k_{j1}, \ldots, k_{jb_j-1}$ be the block sizes in D_j. Let

$$r_j = (r_{j0}, r_{j1}, \ldots, r_{js_j-1})', \qquad k_j = (k_{j0}, k_{j1}, \ldots, k_{jb_j-1})',$$

$$R_j = \mathrm{Diag}(r_{j0}, r_{j1}, \ldots, r_{js_j-1}), \qquad K_j = \mathrm{Diag}(k_{j0}, k_{j1}, \ldots, k_{jb_j-1}).$$

The elements of r_j or k_j are not necessarily equal. The usual C-matrix of D_j is then (cf. Raghavarao (1971)) given by, say,

$$C_j = R_j - N_j K_j^{-1} N_j'. \tag{2.1}$$

The efficiency with which a treatment contrast with the $s_j \times 1$ coefficient vector u_j is estimated in D_j is defined as

$$e_j(u_j) = \begin{cases} u_j' R_j^{-1} u_j / u_j' C_j^- u_j & \text{if the contrast is estimable in } D_j, \\ 0 & \text{otherwise,} \end{cases} \tag{2.2}$$

where C_j^- is any generalized (g-) inverse of C_j. Clearly, (2.2) is based on a comparison of D_j with the corresponding (unblocked) completely randomized design having the same replication numbers as D_j. Note that (2.2) remains the same for every choice of the g-inverse C_j^-.

Let D be an $s_1 \times s_2 \times \cdots \times s_m$ factorial design with incidence matrix

$$N = \bigotimes_{j=1}^{m} N_j, \tag{2.3}$$

where $\otimes$ denotes Kronecker product. Let $v = \prod s_j$, $b = \prod b_j$. Then the replication numbers and block sizes in D are elements of the $v \times 1$ and $b \times 1$ vectors $r = r_1 \otimes \cdots \otimes r_m$ and $k = k_1 \otimes \cdots \otimes k_m$ respectively. Note that neither the replication numbers nor the block sizes in D are necessarily equal. Let R and K be $v \times v$ and

$b\times b$ diagonal matrices with diagonal elements given by the elements of the vectors r and k repectively. Then by (2.1), (2.3), the C-matrix of D equals

$$C = R - NK^{-1}N' = \bigotimes_{j=1}^{m} R_j - \bigotimes_{j=1}^{m} (R_j - C_j). \tag{2.4}$$

Let τ be the $v\times 1$ vector of treatment effects in D, arranged lexicographically. Analogously to (2.2), the efficiency with which a treatment contrast $u'\tau$ is estimated in D is defined as

$$e(u) = \begin{cases} u'R^{-1}u/u'C^{-}u & \text{if the contrast is estimable in } D, \\ 0 & \text{otherwise,} \end{cases} \tag{2.5}$$

C^{-} being any g-inverse of C. It may be seen that in D all main effect contrasts are estimable if and only if each of $D_1,\dots,D_m$ is connected. It is, therefore, assumed hereafter that each of $D_1,\dots,D_m$ is connected. This implies the connectedness of D and ensures the existence of the matrix inverses used in this paper.

3. Lower bounds for interaction efficiencies

The following lemmas will be helpful. The proof of the first lemma is straightforward while that of the second lemma follows essentially along the line of Rao (1973, pp. 70). The column space of any matrix A will be denoted by $\mathscr{M}(A)$.

Lemma 3.1. *For $1\le j\le m$, let A_j, B_j be non-negative definite (n.n.d.) matrices such that $A_j - B_j$ is n.n.d. Then*

$$\bigotimes_{j=1}^{m} A_j - \bigotimes_{j=1}^{m} B_j$$

is n.n.d.

Lemma 3.2. *Let A, B be n.n.d. matrices such that $A-B$ is n.n.d. Then $\mathscr{M}(B)\subseteq\mathscr{M}(A)$ and for every vector $u\in\mathscr{M}(B)$,*

$$u'B^{-}u \ge u'A^{-}u,$$

where A^{-}, B^{-} are any g-inverses of A, B respectively.

For $1\le j\le m$, let u_j be any $s_j\times 1$ non-null vector satisfying $u_j'1_j = 0$. Let T be the set of all m-component non-null binary vectors. For any $x=(x_1,\dots,x_m)\in T$, define the $v\times 1$ vector

$$u^{x} = \bigotimes_{j=1}^{m} u_j^{x_j}, \tag{3.1}$$

where $u_j^{x_j} = u_j$ if $x_j = 1$, $= 1_j$ if $x_j = 0$. Then $u^{x'}\tau$ represents a typical contrast belonging to the factorial effect $F_1^{x_1} \cdots F_m^{x_m}$ (cf. Mukerjee (1979)). The following theorem sets a lower bound for $e(u^x)$ and demonstrates that even in a non-equireplicate setting, high efficiencies with respect to contrasts belonging to factorial effects in D can be ensured by suitably choosing the initial varietal designs $D_1, \ldots, D_m$.

Theorem 3.1. *$e(u^x) \geq \max_{j: x_j = 1} e_j(u_j)$, for each $x \in T$.*

Proof. For $1 \leq j \leq m$, let

$$L_j = \bigotimes_{f=1}^{m} L_{jf}, \qquad W_j = \bigotimes_{f=1}^{m} W_{jf}, \tag{3.2a}$$

where

$$L_{jf} = W_{jf} = R_f \quad \text{if } f \neq j; \qquad L_{jj} = C_j, \quad W_{jj} = R_j - C_j. \tag{3.2b}$$

Note that for each j,

$$L_j = \bigotimes_{f=1}^{m} R_f - W_j,$$

so that by (2.4),

$$C - L_j = W_j - \bigotimes_{f=1}^{m} (R_f - C_f), \tag{3.3}$$

which is n.n.d. by (3.2) and Lemma 3.1.

Consider now any $x = (x_1, \ldots, x_m) \in T$. Without loss of generality, let $x_1 = 1$. Then by (3.1), (3.2), $u^x \in \mathcal{M}(L_1)$. Since by (3.3), $C - L_1$ is n.n.d., it follows from Lemma 3.2 that

$$\begin{aligned} u^{x\prime} C^- u^x \leq u^{x\prime} L_1^- u^x &= u^{x\prime}(C_1^- \otimes R_2^{-1} \otimes \cdots \otimes R_m^{-1}) u^x \\ &= (u_1' C_1^- u_1) \times \left[\prod_{j=2}^{m} (u_j^{x_j})' R_j^{-1} u_j^{x_j} \right], \end{aligned} \tag{3.4}$$

using (3.1), (3.2). But by (3.1), noting that $x_1 = 1$,

$$u^{x\prime} R^{-1} u^x = (u_1' R_1^{-1} u_1) \times \left[\prod_{j=2}^{m} (u_j^{x_j})' R_j^{-1} u_j^{x_j} \right].$$

Hence by (2.2), (2.5), (3.4), $e(u^x) \geq e_1(u_1)$. Similarly, it may be seen that $e(u^x) \geq e_j(u_j)$ for every j such that $x_j = 1$. This completes the proof.

Remark. Theorem 3.1 extends the basic ideas in Gupta (1986) and Mukerjee (1986) to a non-equireplicate set-up. Since the initial designs $D_1, \ldots, D_m$ are left quite arbitrary, the method of Kronecker product is capable of generating factorial designs with a wide range of parameter values. Moreover, by Theorem 3.1, in the factorial designs so constructed the efficiencies with respect to contrasts of interest may be kept high by an appropriate choice of $D_1, \ldots, D_m$. In fact, as examples reveal, very often one gets the satisfying observation that the actual value of $e(u^x)$ is much higher than the lower bound given in the theorem. Theorem 3.1 holds good even when one consider designs for multiway elimination of heterogeneity. This follows because in such a setting the matrices corresponding to those in (3.3) remain n.n.d. The details, which involve use of projection operators along the line of Mukerjee and Sen (1988), are omitted here.

4. A computation of C^-

It may be seen through examples that non-equireplicate Kronecker factorials rarely have OFS in the sense that they do not satisfy the necessary and sufficient condition for OFS stated in Mukerjee (1979). Still then, a method for computing a g-inverse of C, which does not require the inversion of large matrices, is available.

For $1 \le j \le m$, let Z_j be an $(s_j - 1) \times s_j$ matrix such that $(q_j r_j, Z_j')'$ is orthogonal, where $q_j = (r_j' r_j)^{-1/2}$. For $x = (x_1, \ldots, x_m) \in T$, define

$$Z_x = \bigotimes_{j=1}^{m} Z_j^{x_j}, \tag{4.1a}$$

where

$$Z_j^{x_j} = \begin{cases} Z_j & \text{if } x_j = 1, \\ 1_j' & \text{if } x_j = 0. \end{cases} \tag{4.1b}$$

Let $Z = (\ldots, Z_x', \ldots)'_{x \in T}$ (e.g., for $m = 2$, $Z = (Z_{01}', Z_{10}', Z_{11}')'$), $1 = 1_1 \otimes \cdots \otimes 1_m$, $Z^* = (1, Z')'$.

Lemma 4.1. *The $v \times v$ matrix Z^* is non-singular.*

Proof. Follows by observing that $Z^* = Z_1^* \otimes \cdots \otimes Z_m^*$, where $Z_j^* = (1_j, Z_j')'$ $(1 \le j \le m)$, and that each Z_j^* is non-singular by the definition of Z_j.

Lemma 4.2. *For every $x, y \in T$, $x \ne y$, $Z_x C Z_y' = 0$.*

Proof. Follows from (2.4), (4.1), noting that $Z_j r_j = 0$, $C_j 1_j = 0$ $(1 \le j \le m)$.

Theorem 4.1. *A g-inverse of C is given by $C^- = \sum_{x \in T} Z_x'(Z_x C Z_x')^{-1} Z_x$.*

Proof. Note that for $x \in T$, the non-singularity of $Z_x C Z_x'$ follows as usual from the connectedness of D. Define the $v \times v$ matrices $S = \mathrm{Diag}(0, \ldots, Z_x C Z_x', \ldots)_{x \in T}$, $S^* = \mathrm{Diag}(0, \ldots, (Z_x C Z_x')^{-1}, \ldots)_{x \in T}$. Since $C1 = 0$, by Lemma 4.2, $Z^* C Z^{*\prime} = S$ and hence by Lemma 4.1, $C = Z^{*-1} S Z^{*\prime -1}$. Also, C^- as in the statement of the theorem equals $Z^{*\prime} S^* Z^*$. Hence, clearly $CC^-C = C$, as desired.

Remark. Observe that for each $x \in T$, $Z_x C Z_x'$ is a square matrix of order $\prod (s_j - 1)^{x_j}$

($=a(x)$, say). Hence by Theorem 4.1, the evaluation of C^- requires inversion of matrices of order $a(x)$, $x \in T$. This may lead to computational simplicity since the numbers $a(x)$, $x \in T$, will be much smaller than v, the order of C. It may be seen that Theorem 4.1 remains valid even in a set-up for multiway heterogeneity elimination.

While concluding, we mention the following open problems in the context of non-equireplicate factorials: (a) role of partial OFS (see Chauhan and Dean (1986)), (b) construction in generalized cyclic designs, (c) connexion between efficiency-consistency and OFS (for the corresponding results in the equireplicate case, see Lewis and Dean (1985) and Mukerjee and Dean (1986)) and (d) use of Kronecker-type products for construction in designs of smaller size.

Acknowledgement

The authors are thankful to Professor Sudhir C. Gupta, Northern Illinois University, to the Associate Editor and to a referee for highly constructive suggestions.

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