

## UNIVERSALLY OPTIMAL DESIGNS WITH BLOCKSIZE $p \times 2$ AND CORRELATED OBSERVATIONS

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This paper addresses the problems of determination and construction of universally optimal designs in two-dimensional blocks of size  $p \times 2$ , assuming within-block observations are correlated. Generalized least-squares estimation of treatment contrasts is considered in four fixed block-effects models: (I) with fixed row and column effects, (II) with the row effects only, (III) with the column effects only, and (IV) with neither row nor column effects. For a general dependence structure and  $p = 2$ , optimal designs for Model I are found to coincide with the least-squares optimal designs. For general  $p$ , Models I–IV, and the within-block correlation pattern described by the doubly geometric process, interesting nonbinary block patterns are found for the universally optimal designs. Only for Model IV for small, positive correlations do binary blocks turn out to be best, though binarity with respect to rows or columns is often required. Regardless of the model, the conditions frequently coincide with those for optimal nested row-column designs with uncorrelated errors: one class of these designs is found to be optimal for at least some values of the correlation parameters under all four models, and others are found to be optimal for particular models. The exact form of the blocks for a universally optimum design is found to be quite sensitive to the blocksize and to the magnitude of the correlations under both Models III and IV.

**1. Introduction.** Let there be  $b$  separate blocks of  $pq$  experimental units each, the units in each block being further arranged into  $p$  rows and  $q$  columns. A design  $d$  is an assignment of  $v$  treatments to the  $bpq$  units in this blocked row-column set-up. The problem of optimally choosing the design for estimation of treatment contrasts will be investigated under special cases of the model

$$(1) Y = \mathbf{1}_{bpq} \mu + Z_1 \zeta + Z_2 \rho + Z_3 \gamma + X_d \tau + \varepsilon, \quad \text{cov}(\varepsilon) = I_b \otimes \Sigma = V.$$

Here  $\tau$  is the  $v \times 1$  vector of treatment effects;  $X_d$  is the  $bpq \times v$  plot-treatment design matrix that defines an allocation of treatments to the experimental units; and  $\zeta$ ,  $\rho$ , and  $\gamma$ , some of which may be zero, are vectors of parameters for fixed block effects, fixed row effects within blocks, and fixed column effects within blocks, respectively. Inclusion of  $\rho$  and/or  $\gamma$  in the model depends on the desirability of eliminating systematic heterogeneity in

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the experimental material in the standard directions, and is necessarily application dependent. The matrices  $Z_1$ ,  $Z_2$  and  $Z_3$  are, respectively, the plot-block, plot-row, and plot-column incidence matrices. With plots in row-major order by block,  $\Sigma$  is the within-block covariance matrix of order  $pq$ .  $\Sigma$  and hence  $V$  are positive definite.

The generalized least-squares information matrix  $C_d$  for the estimation of treatment contrasts under (1) and the submodels just mentioned can be written

$$(2) \quad C_d = X_d'V^{-1}X_d - X_d'V^{-1}Z(Z'V^{-1}Z)^{-1}Z'V^{-1}X_d.$$

In (2) the matrix  $Z$  contains as columnwise submatrices the  $Z_i$ 's for which the corresponding nuisance effects are included in the model. For instance, if  $\zeta$ ,  $\rho$  and  $\gamma$  are all included, then  $Z = (Z_1, Z_2, Z_3)$ , while if  $\rho$ , say, is omitted, then  $Z = (Z_1, Z_3)$ .

The matrix  $C_d$ , for any connected design  $d$ , is nonnegative definite with rank  $v - 1$ . Only connected designs are of interest here, as only they provide estimability of all treatment contrasts.  $D(v, b, p, q)$  will denote the class of all designs for  $v$  treatments in  $b$  blocks of size  $p \times q$ . While some members of  $D(v, b, p, q)$  will, depending on the model, be disconnected, these will not be considered as competitors in the design optimality problems to be explored.

Sundry aspects of the problems of optimality and construction of designs under (1) and its submodels have of late been tackled by several authors; see Martin (1982, 1986), Gill and Shukla (1985), Kunert (1987, 1988), Morgan (1990), Morgan and Uddin (1991), Uddin and Morgan (1991), and Martin and Eccleston (1993). A recent overview is provided by Martin (1996). This paper systematically attacks a collection of problems not previously addressed, examining the possibilities according to different choices of  $Z$  and a specified  $\Sigma$ , employing generalized least-squares estimation of treatment contrasts. The method used is that of Kiefer (1975): a design  $d^* \in D(v, b, p, q)$  is universally optimal if (i)  $\text{tr}(C_{d^*}) \geq \text{tr}(C_d)$  for all  $d \in D(v, b, p, q)$ , and (ii)  $C_{d^*}$  is completely symmetric.

It is apparent from a reading of the papers cited above that among the conditions for optimal design under a multiplicity of covariance structures, regardless of which nuisance parameters are included in (1), are requirements for neighbor balancing pairs of treatments in rows, in columns and in diagonals, and for balancing of replication and concurrence counts of treatments on corner plots, on edge plots and on interior plots. It is the complexity of these positional conditions that can make for an unusually messy design problem. However, for  $p = q = 2$  all plots are corner plots, and for blocks of size  $p \times 2$  with  $p \geq 3$ , the interior versus edge plot distinction disappears. These simplifications will be taken advantage of to obtain universally optimal designs in  $p \times 2$  blocks. The  $2 \times 2$  case for the full model (1) is considered in Section 2. Blocks of size  $p \times 2$  for the doubly geometric family of  $\Sigma$  matrices are considered in Section 3. Even with the simplifications afforded by  $q = 2$ , the situation is at times quite intricate, as evidenced by the lengthy notation list in Section 3.1 (of which the reader is duly forewarned!).

Let  $t_1, t_2, \dots, t_y$  be a set of  $y$  nonnegative integers constrained to sum to  $x$ . Two special functions will be needed in Sections 3.4 and 3.5. They are  $h(x, y) = \min \sum_{j=1}^y t_j^2$ , and  $g(x, y) = \min \sum_{j=1}^y [\text{int}^2(t_j/2) + \text{int}^2((t_j + 1)/2)]$ . The values of these functions are

$$h(x, y) = x + (2x - y)\text{int}\left(\frac{x}{y}\right) - y\left[\text{int}^2\left(\frac{x}{y}\right)\right]$$

and

$$2g(x, y) = \begin{cases} h(x, y) + x - y\left[\text{int}\left(\frac{x}{y}\right)\right], & \text{if } \text{int}\left(\frac{x}{y}\right) \text{ is even} \\ h(x, y) + y - x + y\left[\text{int}\left(\frac{x}{y}\right)\right], & \text{if } \text{int}\left(\frac{x}{y}\right) \text{ is odd.} \end{cases}$$

The first of these may be found, for example, in Kiefer (1975). The proof for the second is similar. The value  $h(x, y)$  is achieved by  $t_j$ 's for which  $|t_j - t_{j'}| \leq 1$  for every  $j \neq j'$ . If  $x$  is even, the value  $g(x, y)$  can be achieved by all  $t_j$ 's being even with every  $|t_j - t_{j'}|$  no greater than 2. If  $x$  is odd, it can be achieved by all  $t_j$ 's save one being even, with every  $|t_j - t_{j'}|$  no greater than 2.

Three lemmas for bounds on functions involving  $h$  and  $g$  are used in Section 3. The proofs of these are available from the authors.

**2. Optimal designs with blocksize  $2 \times 2$ .** For blocks of size  $2 \times 2$  and the full model (1), a very strong optimality result will be established. Indeed, even more generality for the dependence structure than allowed by (1) can be incorporated. To this end, denote the covariance matrix for observations in block  $j$  by  $\Sigma_j$ .

**LEMMA 2.1.** *Let  $l = \frac{1}{2}(1, -1, -1, 1)'$  and let  $\Sigma_1, \dots, \Sigma_b$  be any set of positive definite matrices for which  $\theta = l'\Sigma_j l$  does not depend on  $j$ . Then the information matrix for estimation of  $\tau$  in the row and column effects model is  $C_d = (1/\theta)C_d^0$ , where  $C_d^0$  is the information matrix (2) when  $\Sigma \equiv I$ . Hence  $d$  is optimal for generalized least-squares estimation of  $\tau$  iff it is optimal for the ordinary least-squares analysis.*

**PROOF.** Let  $P_0$  and  $P_Z$  be the matrices projecting onto the column spaces of  $l$  and  $Z$ , respectively. Then  $(I - P_Z) = I_b \otimes P_0$ . The projected data vector  $Y^* = (I - P_Z)Y$  has covariance  $\text{cov}(Y^*) = (I - P_Z)\text{diag}(\Sigma_j)(I - P_Z) = \text{diag}(P_0 \Sigma_j P_0) = \theta \text{diag}(P_0) = \theta(I - P_Z)$ , and so the information matrix is  $C_d = [(I - P_Z)X_d]'[\text{var}(Y^*)]^{-1}[(I - P_Z)X_d] = (1/\theta)X_d'(I - P_Z)X_d$ .  $\square$

Hence for a very general setup for the covariance structure, all one need solve is the ordinary least-squares problem.

**DEFINITION.** A design in  $D(v, b, p, q)$  is said to be a *bottom-stratum universally optimum nested row and column design*, or BNRC, if (i) the  $bq$

columns give a balanced block design [Kiefer (1975)] with block size  $p$ , and (ii) within any given block, the treatment assignment in any row is a permutation of the treatment assignment in any other row.

One of the interesting features of BNRC's is that the treatment assignment to blocks is always nonbinary. BNRC's have been studied by Bagchi, Mukhopadhyay, and Sinha (1990), who establish their universal optimality over the class  $D(v, b, p, q)$  for the model (1) with  $\Sigma = \sigma^2 I_{pq}$ , and by Morgan and Uddin (1993) and Chang and Notz (1994).

**THEOREM 2.2.** *For the row and column effects model with blockwise covariance matrices  $\Sigma_j$  satisfying the condition of Lemma 2.1, a BNRC in  $D(v, b, 2, 2)$  is universally optimum.*

More generally than Theorem 2.2 for any criterion  $\Phi$ , if  $d^* \in D(v, b, 2, 2)$  is  $\Phi$ -optimal when  $\Sigma = \sigma^2 I_4$ , then it is  $\Phi$ -optimal when the  $\Sigma_j$  are as specified in Lemma 2.1.

### 3. Optimal designs with blocksize $p \times 2$ and doubly geometric errors.

3.1. *Models and information matrices.* Although optimality conditions for a general dependence structure such as considered for blocks of size  $2 \times 2$  would certainly be desirable, that approach does not allow for compact and comprehensive mathematical results when the block size increases. The initial problems of finding  $\Sigma^{-1}$  and a generalized inverse of  $(Z'V^{-1}Z)$ , needed to determine  $C_d$ , are not even tractable. So the remainder of this paper will deal with a manageable and frequently studied parametric family of covariance matrices. With plots in row-major order, the covariance pattern of the doubly geometric error process [Martin (1979)] is

$$(3) \quad \Sigma = \frac{\sigma^2}{(1-\alpha^2)(1-\beta^2)} \begin{pmatrix} 1 & \alpha & \alpha^2 & \cdots & \alpha^{p-1} \\ \alpha & 1 & \alpha & \cdots & \alpha^{p-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha^{p-1} & \alpha^{p-2} & \alpha^{p-3} & \cdots & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix}$$

where  $\alpha$  and  $\beta$  are the immediate column and row correlations ( $|\alpha|, |\beta| < 1$ ). For the doubly geometric  $\Sigma$ , four models will be considered in turn for the expected value portion of (1):

$$\text{Model I: } E(Y) = 1_{b_{pq}} \mu + Z_1 \zeta + Z_2 \rho + Z_3 \gamma + X_d \tau,$$

$$\text{Model II: } E(Y) = 1_{b_{pq}} \mu + Z_1 \zeta + Z_2 \rho + X_d \tau,$$

$$\text{Model III: } E(Y) = 1_{b_{pq}} \mu + Z_1 \zeta + Z_3 \gamma + X_d \tau,$$

$$\text{Model IV: } E(Y) = 1_{b_{pq}} \mu + Z_1 \zeta + X_d \tau.$$

Model I will be the topic of Section 3.3, Model II of Section 3.2, Model III of Section 3.5 and Model IV of Section 3.4 (the reasons for this ordering will

soon become apparent). Before proceeding to those sections, the information matrices for each model will be given. Their specification will require the following notation. For each  $p \times 2$  block, the plots in positions (1, 1), (1, 2), ( $p$ , 1) and ( $p$ , 2) are referred to as *end* plots and the remaining plots as *interior* plots. First defined are the various neighbor count matrices:

- $N^C = v \times v$  matrix ( $N_{ii'}^C$ ) where  $N_{ii'}^C$  is the number of plots containing treatment  $i$  for which it is immediately neighbored by  $i'$  in columns;  
 $N^D = v \times v$  matrix ( $N_{ii'}^D$ ) where  $N_{ii'}^D$  is the number of plots containing treatment  $i$  for which it is immediately neighbored by  $i'$  in diagonals;  
 $N_E^R = v \times v$  matrix ( $N_{Eii'}^R$ ) where  $N_{Eii'}^R$  is the number of end plots containing treatment  $i$  for which its row neighbor is  $i'$ ;  
 $N_I^R = v \times v$  matrix ( $N_{Iii'}^R$ ) where  $N_{Iii'}^R$  is the number of interior plots containing treatment  $i$  for which its row neighbor is  $i'$ ;  
 $N^R = N_E^R + N_I^R = v \times v$  matrix ( $N_{ii'}^R$ ) where  $N_{ii'}^R$  is the number of plots containing treatment  $i$  for which its row neighbor is  $i'$ .

The diagonal entries of each of the neighbor count matrices must be even, since for each plot containing  $i$  with itself as a neighbor, that neighboring plot is another such plot:

- $C_E^0 =$  least-squares information matrix of the incomplete block design with  $2b$  blocks of size 2 given by the  $2b$  end rows of the  $b$  blocks;  
 $C_I^0 =$  least-squares information matrix of the incomplete block design with  $(p-2)b$  blocks of size 2 given by the  $(p-2)b$  interior rows of the  $b$  blocks;  
 $r_{Ejh} = v \times 1$  column vector ( $r_{Ejhi}$ ) where  $r_{Ejhi}$  is the replication of treatment  $i$  in the two end plots of column  $h$  of the  $j$ th block;  
 $r_{Ijh} = v \times 1$  column vector ( $r_{Ijhi}$ ) where  $r_{Ijhi}$  is the replication of treatment  $i$  in the  $p-2$  interior plots of column  $h$  of the  $j$ th block;  
 $R_E^\delta = v \times v$  diagonal matrix for which the  $i$ th diagonal element is the replication total of treatment  $i$  in the  $4b$  end plots of the  $b$  blocks;  
 $T_j = r_{Ej1} - r_{Ej2} + (1-\alpha)(r_{Ij1} - r_{Ij2})$ ,  $r_{Ij} = r_{Ij1} + r_{Ij2}$  and  $r_{Ej} = r_{Ej1} + r_{Ej2}$ .

Although all of the just-defined matrices and vectors certainly depend on the design  $d$ , to ease the notation, the explicit expression of that dependence has been suppressed.

Now for  $d \in D(v, b, p, 2)$ , let  $C_d^{(1)}, C_d^{(2)}, C_d^{(3)}$  and  $C_d^{(4)}$  be the information matrices for generalized least-squares estimation of treatment contrasts under Models I to IV, respectively. Let  $f(\alpha, p) = 2\alpha + p(1-\alpha)$ . With the above notation,

$$C_d^{(2)} = (1 + \beta) \left[ (1 + \alpha^2) C_I^0 + C_E^0 - \frac{\alpha}{2} (N^C - N^D) \right],$$

$$C_d^{(1)} = C_d^{(2)} - \frac{(1-\alpha)(1+\beta)}{2f(\alpha, p)} \sum_{j=1}^b T_j T_j',$$

$$C_d^{(4)} = (1 + \alpha^2)X'_d X_d - \alpha^2 R_E^\delta + \alpha\beta N^D - \alpha N^C - \beta N^R - \alpha^2 \beta N_I^R \\ - \frac{(1 - \alpha)(1 - \beta)}{2f(\alpha, p)} \sum_{j=1}^b [r_{Ej} + (1 - \alpha)r_{Ij}][r_{Ej} + (1 - \alpha)r_{Ij}]', \\ C_d^{(3)} = C_d^{(4)} - \frac{(1 - \alpha)(1 + \beta)}{2f(\alpha, p)} \sum_{j=1}^b T_j T_j'.$$

The task is to find conditions for maximal trace and complete symmetry of these  $C$ -matrices. Using  $\leq$  in the sense of the nnd ordering, since  $\sum_{j=1}^b T_j T_j'$  is nonnegative definite, they satisfy  $C_d^{(1)} \leq C_d^{(2)}$  and  $C_d^{(3)} \leq C_d^{(4)}$ , with equality in both cases if and only if the design  $d$  satisfies  $T_j = 0$  for all  $j$ . A sufficient condition for this is

$$(4) \quad r_{Ij1} = r_{Ij2} \quad \text{and} \quad r_{Ej1} = r_{Ej2} \quad \text{for all } j;$$

that is, the treatment in the end (interior) plots of the first column of any block are a permutation of the treatments in the end (interior) plots of the second column of the same block.

Thus a design  $d$  which is optimal under Model II and satisfies (4) is also optimal under Model I, and a design optimal under Model IV satisfying (4) is also optimal under Model III. To take advantage of these relationships, the maximal trace and complete symmetry problems will be addressed in this order:  $C_d^{(2)}$ ,  $C_d^{(1)}$ ,  $C_d^{(4)}$ ,  $C_d^{(3)}$ . In each case, the expressions involving interior plots and interior rows should be ignored when  $p = 2$ .

**3.2. Universal optimality under Model II.** Of the four, Model II gives the simplest universal optimality conditions. Obviously  $\text{tr}(C_I^0)$  and  $\text{tr}(C_E^0)$  are maximized if the rows are binary. Also,  $\text{tr}(N^C - N^D)$  is minimized if no like neighbors occur in columns and only like neighbors occur in diagonals, and  $\text{tr}(N^C - N^D)$  is maximized if only like neighbors occur in columns while no like neighbors occur in diagonals. So regardless of  $\beta$ ,  $\text{tr}(C_d^{(2)})$  is maximized for  $\alpha > 0$  if and only if each block of  $d$  is of the form

$$(5) \quad \begin{pmatrix} a & b & a & b & \cdots \\ b & a & b & a & \cdots \end{pmatrix}',$$

and for  $\alpha < 0$  if and only if each block of  $d$  is of the form

$$(6) \quad \begin{pmatrix} a & a & \cdots & a \\ b & b & \cdots & b \end{pmatrix}'.$$

In each case, complete symmetry of  $C_d^{(2)}$  is achieved if one such block is constructed for each unordered pair of treatments.

**THEOREM 3.1.** *Let  $d_1^*$  have a block of the form (5) for each unordered pair of treatments. Let  $d_2^*$  have a block of the form (6) for each unordered pair of*

treatments. Then for Model II,  $d_1^*$  is universally optimal over  $D(v, b, p, 2)$  when  $\alpha > 0$ , and  $d_2^*$  is universally optimal when  $\alpha < 0$ .

3.3. *Universal optimality under Model I.* This section investigates universal optimality under Model I for  $p \geq 3$ ; the case  $p = 2$  is covered by Theorem 2.2. If  $p$  is even, the design  $d_1^*$  of Theorem 3.1 satisfies (4), settling this case.

**THEOREM 3.2.** *The design  $d_1^*$  of Theorem 3.1 is universally optimal over  $D(v, b, p, 2)$  under Model I for all even  $p \geq 4$  when  $\alpha > 0$ , and for all  $\alpha$  when  $p = 2$ .*

The designs  $d_1^*$  for odd  $p$  and  $d_2^*$  do not satisfy (4). This makes it more difficult to identify designs  $d$  which maximize  $\text{tr}(C_d^{(1)})$ . In particular, derivation of conditions for maximum trace requires paying close attention to the diagonal neighbor counts  $N_{ii}^D$ . The following concepts will be useful in this regard, both here and again in Sections 3.4 and 3.5.

For each block, define two sets of  $p$  plots, called diagonals, identified by row-column positions  $\{(1, a_1), (2, a_2), \dots, (p, a_p)\}$  and  $\{(1, a_2), (2, a_3), \dots, (p, a_{p+1})\}$ , where  $a_j = 1$  if  $j$  is odd and  $a_j = 2$  if  $j$  is even. Take these to be ordered sets, so that they are the two lists of consecutive, diagonally neighboring plots in any block.

The treatment assignment to a diagonal defines a collection of diagonal strings, each string being a set of consecutive plots containing the same treatment. For instance, in the  $9 \times 2$  block

$$(7) \quad \begin{pmatrix} 1 & 4 & 2 & 4 & 2 & 4 & 3 & 5 & 2 \\ 3 & 1 & 4 & 2 & 4 & 2 & 5 & 2 & 5 \end{pmatrix}'$$

the diagonal treatment assignments are  $\{1, 1, 2, 2, 2, 2, 3, 2, 2\}$  and  $\{3, 4, 4, 4, 4, 5, 5, 5\}$ , containing four and three strings, respectively. Define the *string pattern* to be the list of the lengths of the strings in the diagonal; for (7) the string patterns are  $(2, 4, 1, 2)$  and  $(1, 5, 3)$ .

Next defined are the designs which will be the subject of Theorem 3.3. As in Theorem 3.2,  $d_1^*$  is a design which has, for each unordered pair  $a$  and  $b$  of treatments, a block of the form (5). Let  $d_3^*$  be a design having a block (8) for each of the ordered triplets  $(a, b, c)'$  given by the columns of a three-rowed semibalanced array of strength 2:

$$(8) \quad \left( \begin{array}{ccc|ccc|ccc} \overbrace{a & b & \dots & a}^{n_1 \text{ columns}} & \overbrace{c & a & \dots & c}^{n_2 \text{ columns}} & \overbrace{b & c & \dots & b}^{n_3 \text{ columns}} \\ \hline a & b & \dots & a & c & a & \dots & c & b & c & \dots & b \\ b & a & \dots & b & a & c & \dots & a & c & b & \dots & c \end{array} \right)'$$

Here the  $n_i$ 's are odd and  $n_1 + n_2 + n_3 = p$ .

**THEOREM 3.3.** *For Model I with  $\alpha > 0$ , let  $p$  be odd. Then the design  $d_1^*$  is universally optimal over  $D(v, b, p, 2)$  if  $p \geq [(1 - 2\alpha)(1 + 3\alpha)]/[2\alpha(1 - \alpha)]$ . Otherwise  $d_3^*$  is universally optimal.*

**PROOF.** Complete symmetry of  $C_{d_1^*}^{(1)}$  and  $C_{d_3^*}^{(1)}$  is easily checked, so the result is proved by comparing the trace of one block of the proposed designs with that of one block of an arbitrary design. The contribution of the first block of a design  $d$  to  $\text{tr}(C_d)$ , after removal of the common factor  $(1 + \beta)$ , will be denoted  $\text{tr}_1(C_d)$ . For the proposed designs,

$$\begin{aligned} \text{tr}_1(C_{d_1^*}^{(1)}) &= p + (p - 2)\alpha^2 + 2(p - 1)\alpha - \frac{(1 + \alpha)^2(1 - \alpha)}{f(\alpha, p)}, \\ \text{tr}_1(C_{d_3^*}^{(1)}) &= p + (p - 2)\alpha^2 + 2(p - 2)\alpha - \frac{\alpha^2(1 - \alpha)}{f(\alpha, p)}, \end{aligned}$$

while for any design  $d$ , using  $\text{tr}_1(C_E^0) = 2 - \frac{1}{2}\text{tr}_1(N_E^R)$ ,

$$\text{tr}_1(C_d^{(1)}) \leq p + (p - 2)\alpha^2 - \frac{1}{2}\text{tr}_1(N_E^R) + \frac{\alpha}{2}\text{tr}_1(N^D - N^C) - \frac{(1 - \alpha)}{2f(\alpha, p)}T_1'T_1.$$

Let  $d$  be a design such that  $\text{tr}_1(N^D - N^C) \geq 4(p - 1) - 2$ . If  $\text{tr}_1(N^D - N^C) > 4(p - 1) - 2$ , then the block is of the form (5). Otherwise, a block of  $d$  must have two disjoint diagonal string patterns  $(p)$  and  $(n_1, n_2)$ , where, since  $p$  is odd, exactly one of  $n_1$  and  $n_2$  is odd. It follows that  $T_1'T_1 = 2(1 + \alpha + \alpha^2)$  and thus  $\text{tr}_1(C_{d_1^*}^{(1)}) \geq \text{tr}_1(C_d^{(1)})$ .

If  $d$  satisfies  $\text{tr}_1(N^D - N^C) \leq 4(p - 1) - 6$ , then  $\text{tr}_1(C_d^{(1)}) \leq p + (p - 2)\alpha^2 + (2p - 5)\alpha \leq \text{tr}_1(C_{d_3^*}^{(1)})$ , which rules out this competitor.

So consider any design  $d$  with  $\text{tr}_1(N^D - N^C) = 4(p - 1) - 4$ . Ruling out  $\text{tr}_1(N^C) = 4$  as combinatorially impossible leaves two ways in which this can happen, each of which will be shown to be no better than  $d_1^*$ , which has this same value of  $\text{tr}_1(N^D - N^C)$ .

First, suppose that  $\text{tr}_1(N^D) = 4(p - 1) - 2$  with  $\text{tr}_1(N^C) = 2$ . In this case, the block of a competing design must have diagonal string patterns of  $(p)$  and  $(p - 1, 1)$ , where the strings of length 1 and  $p$  contain the same treatment. For this pattern,  $T_1'T_1 = 2\alpha^2$  and  $\text{tr}_1(N_E^R) = 2$ , while  $T_1'T_1 = 2(1 + \alpha)^2$  for  $d_1^*$ , so  $\text{tr}_1(C_{d_1^*}^{(1)}) \geq \text{tr}_1(C_d^{(1)})$ .

So suppose that  $\text{tr}_1(N^D) = 4(p - 1) - 4$  with  $\text{tr}_1(N^C) = 0$ . Writing  $\text{tr}_{11}(N^D)$  and  $\text{tr}_{12}(N^D)$  for the contribution of diagonals 1 and 2 to  $\text{tr}_1(N^D)$ , there are two possibilities: (i)  $\text{tr}_{11}(N^D) = 2(p - 1)$ ,  $\text{tr}_{12}(N^D) = 2(p - 1) - 4$ ,  $\text{tr}_1(N^C) = 0$ ; and (ii)  $\text{tr}_{11}(N^D) = 2(p - 1) - 2$ ,  $\text{tr}_{12}(N^D) = 2(p - 1) - 2$ ,  $\text{tr}_1(N^C) = 0$ . First consider (i). In this case, the two diagonals must have disjoint treatments with two diagonal string patterns  $(p)$  and  $(n_1, n_2, n_3)$  where the treatments in the second diagonal may be taken as (i'):  $n_1$   $a$ 's,  $n_2$   $b$ 's and  $n_3$   $c$ 's or as (i''):  $n_1$   $a$ 's,  $n_2$   $b$ 's and  $n_3$   $a$ 's. Note that  $n_i$ 's need not be the same in (i') and (i''). The values of  $T_1'T_1$  according to the parities of the  $n_i$ 's, subject to  $n_1 + n_2 + n_3 = p$ , are given here.

$n_1$	$n_2$	$n_3$	$T'_1 T_1$ for case (i')	$T'_1 T_1$ for case (i'')
even	even	odd	$2(1 + \alpha)^2$	$2(1 + \alpha + \alpha^2)$
even	odd	even	$2 + 6\alpha^2$	$2 + 2\alpha + 3\alpha^2$
odd	even	even	$2(1 + \alpha)^2$	$2(1 + \alpha + \alpha^2)$
odd	odd	odd	$6 + 2\alpha^2$	$3 + (1 + \alpha)^2$ .

In each case,  $\text{tr}_1(C_{d_i^*}^{(1)}) \geq \text{tr}_1(C_{d_1}^{(1)})$ . A similar enumeration disposes of case (ii).  $\square$

The construction used for  $d_3^*$  of Theorem 3.3 should be compared to the technique used by Martin and Eccleston (1993), page 81. Theirs is a map of the columns of a  $2p$ -rowed semibalanced array to a  $p \times 2$  binary block. The important change here is to start with a maximum trace block, from which the development according to the semibalanced array gains complete symmetry and hence universal optimality. The number of rows required of the array equals the number of distinct treatments in the maximum trace block (being three for  $d_3^*$ ). A definition and references for semibalanced arrays may be found in Martin and Eccleston (1991), pages 71–72.

For  $\alpha < 0$ , only a result for even  $p$  will be stated, which will require two designs,  $d_4^*$  and  $d_5^*$ . The design  $d_4^*$  is found by forming the block (9) on each of the  $v(v-1)/2$  unordered pairs of treatments, and  $d_5^*$  is found by forming the block (10) on each of the ordered triples  $(a, b, c)'$  given by the columns of a three-rowed semibalanced array of strength 2 [these arrays always exist with minimal index; see Morgan and Chakravarti (1988), page 1214]. Again, complete symmetry is immediate. The proof of the next theorem thus amounts to showing that the blocks (9) and (10) are of maximal trace under the stated conditions:

$$(9) \quad \left( \begin{array}{c|c} \overbrace{a \ a \ \cdots \ a}^{p/2 \text{ columns}} & \overbrace{b \ b \ \cdots \ b}^{p/2 \text{ columns}} \\ \hline \overbrace{b \ b \ \cdots \ b}^{p/2 \text{ columns}} & \overbrace{a \ a \ \cdots \ a}^{p/2 \text{ columns}} \end{array} \right)',$$

$$(10) \quad \left( \begin{array}{c|c} \overbrace{a \ a \ \cdots \ a \ a}^{p/2 \text{ columns}} & \overbrace{b \ b \ \cdots \ b \ b}^{p/2 \text{ columns}} \\ \hline \overbrace{b \ b \ \cdots \ b \ c}^{p/2 \text{ columns}} & \overbrace{c \ a \ a \ \cdots \ a}^{p/2 \text{ columns}} \end{array} \right)'.$$

**THEOREM 3.4.** *For Model I with  $\alpha < 0$ , let  $p$  be even. Then the design  $d_4^*$  is universally optimal over  $D(v, b, p, 2)$  if  $p \leq -[2\alpha^2 + 3(1 - \alpha)^3]/[\alpha(1 - \alpha)]$ . Otherwise,  $d_5^*$  is universally optimal.*

The condition implies that  $p$  must be at least 13 for  $d_5^*$  to be better for any  $\alpha$ . Theorem 3.4 is offered as an example of how different is the design situation when  $\alpha$  is negative. Its proof involves a fairly painstaking examination of a longer list of cases than in the proof of Theorem 3.3, so is omitted here. For odd  $p$  and negative  $\alpha$ , we mention only that the form of the

maximal trace block depends in a more complex way on  $p$ , and involves more than a choice between two competitors as in Theorem 3.4.

3.4. *Universal optimality under Model IV.* The simplest of the models to specify, Model IV with block effects only, induces more complicated conditions than either of the models thus far treated. To ease the situation somewhat, only  $\alpha > 0$ ,  $\beta > 0$  and  $2p \leq v$  will be considered. The key to identifying a maximal trace block lies in a close examination of the *diagonal strings* as defined in Section 3.3.

First write  $V_j = r_{Ej} + (1 - \alpha)r_{Ij}$ , so that

$$\begin{aligned} \text{tr}(C_d^{(4)}) &= 2pb(1 + \alpha^2) - 4b\alpha^2 - \alpha \text{tr}(N^C) \\ &\quad - \beta \text{tr}(N^R) - \alpha^2\beta \text{tr}(N_I^R) + H_d, \end{aligned}$$

where  $H_d = \alpha\beta \text{tr}(N^D) - ((1 - \alpha)(1 - \beta)/2f(\alpha, p))\sum_{j=1}^b V_j' V_j$ . Note that if a given diagonal contains  $s$  strings, then its contribution to  $\text{tr}(N^D)$  is  $2(p - s)$ . Given any block and its contribution to  $\text{tr}(N^D)$ , since  $2p \leq v$ , it is always possible to make its two diagonals contain disjoint sets of treatments, and to make strings within each diagonal be composed of separate sets of treatments, without changing that contribution. Doing this minimizes the sum of its like row and column neighbor counts (by making them both zero), and minimizes  $V_j' V_j$  subject to the given string patterns of the two diagonals. So  $\text{tr}(C_d^{(4)}) \leq 2pb(1 + \alpha^2) - 4b\alpha^2 + H_d$ , with equality achieved by disjoint diagonals of disjoint strings in each block, and  $\text{tr}(C_d^{(4)})$  is thus maximized by appropriate choice of string patterns for the diagonals. Given that the two diagonals of each block are disjoint,  $H_d$  can be written  $H_d = \alpha\beta \sum_{i=1}^v \sum_{j=1}^b \sum_{l=1}^2 N_{iijl}^D - ((1 - \alpha)(1 - \beta)/2f(\alpha, p))\sum_{j=1}^b \sum_{l=1}^2 V_{jl}' V_{jl}$ , where  $N_{iijl}^D$  is the diagonal like-neighbor count for treatment  $i$  in diagonal  $l$  of block  $j$ , and  $V_{jl} = \bar{r}_{Ejl} + (1 - \alpha)\bar{r}_{Ijl}$ . Here  $\bar{r}_{Ejl}$  and  $\bar{r}_{Ijl}$  are the end and interior replication vectors for treatments in diagonal  $l$  of block  $j$  (as distinguished from the  $r_{Ejl}$  and  $r_{Ijl}$ , which are for column  $l$ ). So to maximize  $H_d$ , it is sufficient for each  $j$  and  $l$  to maximize  $H_{djl} = \alpha\beta \sum_{i=1}^v N_{iijl}^D - ((1 - \alpha)(1 - \beta)/2f(\alpha, p))V_{jl}' V_{jl}$ . An *optimum string pattern* is a pattern of disjoint strings that maximizes  $H_{djl}$ . The goal is to find an optimum string pattern. Maximization of trace has been reduced to the investigation of treatment assignment to a single diagonal.

A pattern of disjoint strings is said to be of type  $(s, l_1, l_2)$  if it consists of  $s$  strings and if the strings containing the two end plots are of lengths  $l_1$  and  $l_2$ , respectively. Take  $l_1 \geq l_2$ . If there is only one string, the type is  $(1, p, 0)$ . In (7), one of the diagonals is composed of disjoint strings, and its pattern is type  $(3, 3, 1)$ .

Given a diagonal of disjoint strings of type  $(s, l_1, l_2)$ , with pattern  $(l_1, t_1, t_2, \dots, t_{s-2}, l_2)$  and  $l_2 \geq 1$ , its value of  $V_{jl}' V_{jl}$  is  $(1 - \alpha)^2[(l_1 - 1)^2 + (l_2 - 1)^2 + \sum_{h=1}^{s-2} t_h^2] + 2(1 - \alpha)(l_1 + l_2 - 2) + 2$ . This quantity is minimized over all patterns of type  $(s, l_1, l_2)$  by minimizing  $\sum_{h=1}^{s-2} t_h^2$  subject to  $\sum_{h=1}^{s-2} t_h = p - l_1 - l_2$ . Using the function  $h$  defined at the end of Section 1, the

minimum value of  $V'_{jl}V_{jl}$  over all string patterns of type  $(s, l_1, l_2)$  and  $l_2 \geq 1$ , denoted  $w(s, l_1, l_2)$ , is

$$w(s, l_1, l_2) = (1 - \alpha)^2 [(l_1 - 1)^2 + (l_2 - 1)^2 + h(p - l_1 - l_2, s - 2)] \\ + 2(1 - \alpha)(l_1 + l_2 - 2) + 2.$$

For  $l_1 = p, l_2 = 0$ , the value is  $w(1, p, 0) = [f(\alpha, p)]^2$ .

LEMMA 3.5.

$$w(s, l_1, l_2) - w(p, 1, 1) \geq \begin{cases} 2(p - s)(1 - \alpha)^2, & \text{if } p \geq 4, \\ 2(p - s)(1 - \alpha), & \text{if } p = 3, \end{cases}$$

for  $1 \leq s \leq p - 1$ , with equality for  $s = p - 1$  and  $l_1 = l_2 = 1$ .

LEMMA 3.6.

$$w(1, p, 0) - w(s, l_1, l_2) \leq \begin{cases} \frac{(s - 1)[f(\alpha, p)]^2}{2}, & \text{if } p \text{ is even,} \\ \frac{(s - 1)[f(\alpha, p)]^2}{2} - \frac{(s - 1)(1 - \alpha)^2}{2}, & \text{if } p \text{ is odd,} \end{cases}$$

for  $2 \leq s \leq p$ , with equality for  $s = 2$  and  $l_1 = \text{int}[(p + 1)/2]$ .

THEOREM 3.7. Under Model IV with  $\alpha > 0$  and  $\beta > 0$ , a binary-block design  $d^*$  in  $D(v, b, p, 2)$ ,  $2p \leq v$ , has maximal trace if and only if

$$\frac{(1 - \alpha)(1 - \beta)}{4\alpha\beta} \geq 1 \quad \text{for } p = 2,$$

$$\frac{(1 - \alpha)^2(1 + \beta)}{2(1 + \alpha)\beta} \geq 1 \quad \text{for } p = 3,$$

$$\frac{(1 - \alpha)^3(1 - \beta) - 4\alpha^2\beta}{2\alpha(1 - \alpha)\beta} \geq p \quad \text{for } p \geq 4.$$

Under these conditions, forming a  $p \times 2$  block on each column of a  $2p$ -rowed semibalanced array gives a universally optimal design.

PROOF. Suppose  $p \geq 4$ . A binary block design  $d^*$  has

$$H_{d^*jl} = -\frac{(1 - \alpha)(1 - \beta)}{2f(\alpha, p)}w(p, 1, 1),$$

while a superior competitor  $d$  would have

$$H_{djl} \leq 2\alpha\beta(p - s) - \frac{(1 - \alpha)(1 - \beta)}{2f(\alpha, p)}w(s, l_1, l_2)$$

for some  $1 \leq s \leq p - 1$ . So by Lemma 3.5,

$$\begin{aligned} & \text{tr}(C_{d^*}) - \text{tr}(C_d) \\ & \geq H_{d^*} - H_d = \sum_j \sum_l (H_{d^*jl} - H_{djl}) \\ & \geq 2b \left\{ -2\alpha\beta(p-s) + \frac{(1-\alpha)(1-\beta)[w(s, l_1, l_2) - w(p, 1, 1)]}{2f(\alpha, p)} \right\} \\ & \geq \frac{2b(p-s)}{f(\alpha, p)} \left[ (1-\alpha)^3(1-\beta) - 4\alpha^2\beta - 2\alpha(1-\alpha)\beta p \right] \geq 0. \end{aligned}$$

The same argument using the latter inequality of Lemma 3.5, and again using the Lemma 3.6 inequality, proves the result for  $p = 3$  and  $p = 2$ .  $\square$

Also, if either  $\alpha$  or  $\beta$  is 0, a binary block will be best. The result for  $p = 2$  with  $\alpha = \beta$  in Theorem 3.7 appears in Martin and Eccleston (1993), page 86.

**THEOREM 3.8.** *Under Model IV with  $\alpha > 0$  and  $\beta > 0$ , the design  $d_1^*$  in  $D(v, b, p, 2)$ ,  $2p \leq v$ , is universally optimum if*

$$\begin{aligned} & \frac{8\alpha\beta}{(1-\alpha)(1-\beta)} \geq f(\alpha, p) \quad \text{for even } p, \\ & \frac{8\alpha\beta}{(1-\alpha)(1-\beta)} + \frac{(1-\alpha)^2}{f(\alpha, p)} \geq f(\alpha, p) \quad \text{for odd } p. \end{aligned}$$

**PROOF.** The proposed design  $d_1^*$  has  $H_{d_1^*jl} = 2\alpha\beta(p-1) - ((1-\alpha) \times (1-\beta)/2f(\alpha, p))w(1, p, 0)$ , while a superior competitor  $d$  would have  $H_{djl}$  as in the proof of Theorem 3.7 for some  $s \geq 2$ . The result follows by comparing  $H_{d_1^*jl}$  and  $H_{djl}$ , arguing as in that proof and using Lemma 3.6  $\square$

Theorems 3.7 and 3.8 cover small and large combinations of the correlations. For other values, a maximum trace design has all blocks composed of two disjoint diagonals with string patterns of type  $(s, l_1, l_2)$ , where the values  $s$ ,  $l_1$  and  $l_2$  maximize

$$(11) \quad 2\alpha\beta(p-s) - \frac{(1-\alpha)(1-\beta)}{2f(\alpha, p)}w(s, l_1, l_2).$$

This is an integer programming problem which, as demonstrated by the two preceding theorems, is quite sensitive to  $p$ ,  $\alpha$  and  $\beta$ . But for given values of these parameters the maximum is easily calculated by computer. Optimum types  $(s, l_1, l_2)$  are displayed for a selected range of the symmetric process (put  $\alpha = \beta$ ) in Table 1. Given the type which maximizes trace, universally optimum designs are simply constructed using the semibalanced array technique. For all  $p$  covered in Table 1, type  $(1, p, 0)$  is optimal for  $\alpha$  of 0.6 and greater.

TABLE 1  
*Optimal string types for Model IV with  $\alpha = \beta$*

$p$	$\alpha$				
	0.1	0.2	0.3	0.4	0.5
3	(3, 1, 1)	(3, 1, 1)	(2, 2, 1)	(1, 3, 0)	(1, 3, 0)
4	(4, 1, 1)	(4, 1, 1)	(2, 2, 2)	(1, 4, 0)	(1, 4, 0)
5	(5, 1, 1)	(5, 1, 1)	(2, 3, 2)	(2, 3, 2)	(1, 5, 0)
6	(6, 1, 1)	(4, 1, 1)	(3, 2, 2)	(2, 3, 3)	(1, 6, 0)
7	(7, 1, 1)	(5, 1, 1)	(3, 2, 2)	(2, 4, 3)	(1, 7, 0)
8	(8, 1, 1)	(5, 1, 1)	(3, 2, 2)	(2, 4, 4)	(1, 8, 0)
9	(9, 1, 1)	(6, 1, 1)	(3, 3, 3)	(2, 5, 4)	(1, 9, 0)
10	(10, 1, 1)	(5, 2, 2)	(3, 3, 3)	(2, 5, 5)	(1, 10, 0)
15	(15, 1, 1)	(7, 2, 2)	(4, 3, 3)	(2, 8, 7)	(2, 8, 7)
20	(20, 1, 1)	(8, 2, 2)	(4, 5, 5)	(3, 6, 6)	(2, 10, 10)

Starting with  $(s, l_1, l_2)$  from Table 1, a diagonal is constructed with end strings of lengths  $l_1$  and  $l_2$  and  $s - 2$  other strings with lengths as equal as possible. This “equal as possible” condition comes from minimizing  $\sum t_j^2$  as explained just before Lemma 3.5. To illustrate, take  $p$  of 7 and  $\alpha$  of 0.2. Each diagonal should contain five strings, the two end strings being of length 1 each, and the other three dividing the remaining five plots as equally as possible. So one maximum track block is

$$\begin{pmatrix} 1 & 7 & 2 & 8 & 3 & 9 & 5 \\ 6 & 2 & 8 & 3 & 9 & 4 & 10 \end{pmatrix}'.$$

3.5. *Universal optimality under Model III.* As was done for Model IV, now take  $\alpha > 0$  and  $\beta > 0$  in Model III. Results roughly paralleling Theorems 3.7 and 3.8 will be derived for even  $p$ . As will be seen, the proofs, aside from a small modification, follow nicely along the lines of the work in Section 3.4. Corresponding work for odd  $p$  is explained after Theorem 3.11.

First, (4) holds for Theorem 3.8 designs when  $p$  is even, and so partially settles the issue.

**THEOREM 3.9.** *Let  $p$  be even with  $2p \leq v$ . Then the design  $d_1^*$  is universally optimal in  $D(v, b, p, 2)$  under Model III with  $\alpha > 0$  and  $\beta > 0$  if  $8\alpha\beta/[(1 - \alpha)(1 - \beta)] \geq f(\alpha, p)$ .*

For  $p = 2$  it can be shown that the Theorem 3.9 result holds for all  $\alpha > 0$  and  $\beta > 0$ .

When (4) cannot be satisfied by a design of Section 3.4, which, save for the designs appearing in Theorem 3.8, is always the case, the current expression for  $C_d^{(3)}$  given in Section 3.1 is not particularly useful. Write  $U_{j1} = r_{Ej1} + (1 - \alpha)r_{Ij1}$  and  $U_{j2} = r_{Ej2} + (1 - \alpha)r_{Ij2}$ . Starting with that expression from

Section 3.1, a simple calculation gives

$$C_d^{(3)} = (1 + \alpha^2)X'_d X_d - \alpha^2 R_E^\delta + \alpha\beta N^D - \alpha N^C - \beta N^R - \alpha^2\beta N_I^R \\ - \frac{(1 - \alpha)(1 - \beta)}{f(\alpha, p)} \sum_{j=1}^b (U_{j1}U'_{j1} + U_{j2}U'_{j2}) - \frac{(1 - \alpha)\beta}{f(\alpha, p)} \sum_{j=1}^b T_j T'_j$$

from which

$$(12) \quad \text{tr}(C_d^{(3)}) \leq 2pb(1 + \alpha^2) - 4b\alpha^2 - \alpha \text{tr}(N^C) \\ - \beta \text{tr}(N^R) - \alpha^2\beta \text{tr}(N_I^R) + G_d$$

where  $G_d = \alpha\beta \text{tr}(N^D) - ((1 - \alpha)(1 - \beta)/f(\alpha, p))\sum_{j=1}^b (U'_{j1}U_{j1} + U'_{j2}U_{j2})$ , and  $\sum_{j=1}^b T'_j T_j$  has been set to zero.

Just as for Model IV (compare  $G_d$  to  $H_d$  of Section 3.4), given any block and its contribution to  $\text{tr}(N^D)$ , it is always possible to make its two diagonals contain disjoint sets of treatments, and to make strings within each diagonal be composed of separate sets of treatments, without changing that contribution. Doing this minimizes the sum of its like row and column neighbor counts, and minimizes  $U'_{j1}U_{j1} + U'_{j2}U_{j2}$  subject to the given string patterns of the two diagonals. So  $\text{tr}(C_d^{(3)}) \leq 2pb(1 + \alpha^2) - 4b\alpha^2 + G_d$ , with equality achieved by disjoint diagonals of disjoint strings in each block, and  $\text{tr}(C_d^{(3)})$  is thus maximized by appropriate choice of string patterns for the diagonals, provided that choice makes (4) hold. Unfortunately, (4) will usually not hold simultaneously with the requirement of disjoint diagonals of disjoint strings, a problem which will temporarily be put on hold. For now, the term involving  $T'_j T_j$  will be ignored and conditions for maximization of  $G_d$  will be found. Then the required adjustment to account for nonzero  $T'_j T_j$  will be made.

Given a diagonal of disjoint strings of type  $(s, l_1, l_2)$ , with pattern  $(l_1, t_1, t_2, \dots, t_{s-2}, l_2)$  and  $l_2 \geq 1$  (and hence  $s > 1$ ), its contribution to  $U'_{j1}U_{j1} + U'_{j2}U_{j2}$  is

$$2\alpha^2 + 2\alpha(1 - \alpha) \left[ \text{int}\left(\frac{l_1 + 1}{2}\right) + \text{int}\left(\frac{l_2 + 1}{2}\right) \right] \\ + (1 - \alpha)^2 \sum_{j=1}^{s-2} \left[ \text{int}^2\left(\frac{t_j}{2}\right) + \text{int}^2\left(\frac{t_j + 1}{2}\right) \right] \\ + (1 - \alpha)^2 \left[ \text{int}^2\left(\frac{l_1}{2}\right) + \text{int}^2\left(\frac{l_2}{2}\right) + \text{int}^2\left(\frac{l_1 + 1}{2}\right) + \text{int}^2\left(\frac{l_2 + 1}{2}\right) \right] \\ \geq 2\alpha^2 + 2\alpha(1 - \alpha) \left[ \text{int}\left(\frac{l_1 + 1}{2}\right) + \text{int}\left(\frac{l_2 + 1}{2}\right) \right] \\ + (1 - \alpha)^2 g(p - l_1 - l_2, s - 2) \\ + (1 - \alpha)^2 \left[ \text{int}^2\left(\frac{l_1}{2}\right) + \text{int}^2\left(\frac{l_2}{2}\right) + \text{int}^2\left(\frac{l_1 + 1}{2}\right) + \text{int}^2\left(\frac{l_2 + 1}{2}\right) \right] \\ = w^*(s, l_1, l_2).$$

For  $s = 1$ , this lower bound value is  $w^*(1, p, 0) = [f(\alpha, p)]^2/2$ .

LEMMA 3.10. Let  $p \geq 4$  be even and, if  $s > 1$ , let  $l_1 \geq l_2 \geq 2$ . Then for  $1 \leq s \leq (p/2) - 1$ ,

$$w^*(s, l_1, l_2) - w^*\left(\frac{p}{2}, 2, 2\right) \geq \begin{cases} 2(p - 2s)(1 - \alpha)^2, & \text{if } p \geq 8, \\ 2(p - 2s)\left[(1 - \alpha)^2 + \frac{\alpha(1 - \alpha)}{2}\right], & \text{if } p = 6, \\ 2(p - 2s)(1 - \alpha), & \text{if } p = 4, \end{cases}$$

with equality at  $s = (p/2) - 1$  and  $(l_1, l_2)$  given by  $(4, 0)$ ,  $(4, 2)$  or  $(2, 2)$ , as  $p = 4$ ,  $p = 6$  or  $p \geq 8$ .

Now a result paralleling Theorem 3.8 can be stated. The required block, to which the semibalanced array construction can be applied, is

$$(13) \quad \begin{pmatrix} a & b & c & d & \cdots \\ b & a & d & c & \cdots \end{pmatrix}'$$

with both diagonal strings of type  $(p/2, 2, 2)$ .

THEOREM 3.11. Under Model III with  $\alpha > 0$  and  $\beta > 0$ , even  $p \geq 4$ , and  $2p \leq v$ , a design  $d^*$  maximizing  $G_d$  in  $D(v, b, p, 2)$ , has only blocks of the form (13) if and only if

$$\begin{aligned} \frac{2(1 - \alpha)^2(1 - \beta) - 2\alpha^2\beta}{\alpha(1 - \alpha)\beta} &> p \quad \text{for } p = 4, \\ \frac{(1 - \alpha)^2(1 - \beta)(2 - \alpha) - 2\alpha^2\beta}{\alpha(1 - \alpha)\beta} &> p \quad \text{for } p = 6, \\ \frac{2(1 - \alpha)^3(1 - \beta) - 2\alpha^2\beta}{\alpha(1 - \alpha)\beta} &> p \quad \text{for } p \geq 8. \end{aligned}$$

Under these conditions, forming a  $p \times 2$  block (13) on each column of a  $p$ -rowed semibalanced array gives a design with efficiency at least

$$1 - \frac{2\alpha^2(1 - \alpha)\beta}{[p(1 + \alpha^2) - 2\alpha^2 + \alpha\beta p]f(\alpha, p) - (1 - \alpha)(1 - \beta)w^*(p/2, 2, 2)}.$$

PROOF. Let  $G_{d,jl}$  be the contribution of diagonal  $l$  in block  $j$  of design  $d$  to  $G_d$ . A design  $d^*$  with all blocks as specified has  $G_{d^*,jl} = \alpha\beta p - ((1 - \alpha) \times (1 - \beta)/f(\alpha, p))w^*(p/2, 2, 2)$ , while a superior competitor  $d$  would have  $G_{d,jl} \leq 2\alpha\beta(p - s) - ((1 - \alpha)(1 - \beta)/f(\alpha, p))w^*(s, l_1, l_2)$  for some  $1 \leq s \leq p$ . It is easy to check that  $w^*(s, l_1, l_2) \geq w^*(p/2, 2, 2)$  for  $s > p/2$ , which rules out these competitors. Also easy is  $w^*(s, l_1, l_2) > w^*(s, 2, 2)$  if  $l_2 = 1$ ,

so for  $s \geq 2$ , assume  $2 \leq l_2 \leq l_1$ . Then by Lemma 3.10 for  $p \geq 8$ ,

$$\begin{aligned} G_{d^*} - G_d &= \sum_j \sum_l (G_{d^*jl} - G_{djl}) \\ &\geq 2b \left\{ -\alpha\beta(p - 2s) \right. \\ &\quad \left. + \frac{(1 - \alpha)(1 - \beta)[w^*(s, l_1, l_2) - w^*(p/2, 2, 2)]}{f(\alpha, p)} \right\} \\ &\geq \frac{2b(p - 2s)}{f(\alpha, p)} [-2\alpha^2\beta + 2(1 - \alpha)^3(1 - \beta) - \alpha(1 - \alpha)\beta p] > 0. \end{aligned}$$

Similar calculations give the maximization result for  $p = 4$  and  $p = 6$ .

The efficiency bound comes from (12), which ignores  $T'_j T_j$ , the value of which is  $4\alpha^2$  for  $d^*$ . Simply compare (12) for  $d^*$ , to the same value minus  $((1 - \alpha)\beta/f(\alpha, p))\sum_j T'_j T_j = (4b\alpha^2(1 - \alpha)\beta/f(\alpha, p))$ .  $\square$

Similar to (11) for Model IV, highly efficient designs for Model III and even  $p$  can be found by using diagonal string patterns of type  $(s, l_1, l_2)$  which maximize

$$(14) \quad 2\alpha\beta(p - s) - \frac{(1 - \alpha)(1 - \beta)}{f(\alpha, p)} w^*(s, l_1, l_2).$$

Whenever the maximizing values  $(s, l_1, l_2)$  have  $l_1$  and  $l_2$  (and hence  $p - l_1 - l_2$ ) all even (this is always the case), the maximum can be achieved by a pattern of disjoint strings all of even length (see the comment regarding the function  $g$  at the end of Section 1), so that  $T^* = T'_j T_j$  takes the value  $4\alpha^2$ . A lower bound for the efficiency is thus 1 minus

$$(15) \quad \frac{(1 - \alpha)\beta T^*/2}{[p(1 + \alpha^2) - 2\alpha^2 + 2\alpha\beta(p - s)]f(\alpha, p) - (1 - \alpha)(1 - \beta)w^*(s, l_1, l_2)}$$

(cf. the bound of Theorem 3.11), where again  $(s, l_1, l_2)$  are the maximizing values of (14). As for (11), maximization of (14) as a general problem is computationally simple although analytically difficult. Maximizing pattern types, and corresponding efficiency lower bounds truncated to three decimal places, are displayed for the symmetric process in Table 2. It is evident that the potential efficiency loss incurred by  $T'_j T_j$  being nonzero is very small. For the range of  $p$  covered in Table 2, string patterns of type  $(1, p, 0)$  are fully efficient for  $\alpha$  of 0.6 and above.

Given the type maximizing (14), a diagonal is constructed by making the  $s - 2$  interior string lengths as equal as possible, subject to their all being even; this is the condition for attaining the value  $g(p - l_1 - l_2, s - 2)$  in  $w^*(s, l_1, l_2)$ . For example, with  $p$  of 18 and  $\alpha$  and  $\beta$  of 0.3, a maximizing string pattern is  $(4, 4, 6, 4)$ . The pattern  $(4, 5, 5, 4)$  gives the same value to  $w^*$ , but inflates  $T'_j T_j$ .

TABLE 2  
String pattern types maximizing (14) for  $\alpha = \beta$ , and Model III efficiencies

$p$	$\alpha$				
	0.1	0.2	0.3	0.4	0.5
4	(2, 2, 2, 0.999)	(2, 2, 2, 0.999)	(2, 2, 2, 0.997)	(1, 4, 0, 1.000)	(1, 4, 0, 1.000)
6	(3, 2, 2, 0.999)	(3, 2, 2, 0.999)	(3, 2, 2, 0.998)	(2, 4, 2, 0.997)	(1, 6, 0, 1.000)
8	(4, 2, 2, 0.999)	(4, 2, 2, 0.999)	(3, 2, 2, 0.999)	(2, 4, 4, 0.998)	(1, 8, 0, 1.000)
10	(5, 2, 2, 0.999)	(5, 2, 2, 0.999)	(3, 4, 2, 0.999)	(2, 6, 4, 0.999)	(1, 10, 0, 1.000)
12	(6, 2, 2, 0.999)	(6, 2, 2, 0.999)	(3, 4, 4, 0.999)	(2, 6, 6, 0.999)	(1, 12, 0, 1.000)
14	(7, 2, 2, 0.999)	(7, 2, 2, 0.999)	(4, 4, 2, 0.999)	(2, 8, 6, 0.999)	(1, 14, 0, 1.000)
16	(8, 2, 2, 0.999)	(8, 2, 2, 0.999)	(4, 4, 4, 0.999)	(2, 8, 8, 0.999)	(2, 8, 8, 0.999)
18	(9, 2, 2, 0.999)	(9, 2, 2, 0.999)	(4, 4, 4, 0.999)	(3, 6, 6, 0.999)	(2, 10, 8, 0.999)
20	(10, 2, 2, 0.999)	(10, 2, 2, 0.999)	(5, 4, 4, 0.999)	(3, 6, 6, 0.999)	(2, 10, 10, 0.999)

For odd  $p$  under Model III, this bounding approach works just the same, though it is not quite as sharp. The difficulty lies in the interplay of the quantities  $w^*(s, l_1, l_2)$  and  $T_j' T_j$ . Unlike for even  $p$ , string patterns maximizing (14) must have one string of odd length, which makes for a larger departure of  $T_j' T_j$  from zero and a correspondingly lower efficiency bound. Table 3 demonstrates by computation that maximizing (14) for disjoint strings is still satisfactory. The efficiencies are from (15) with the value of  $T^*$  depending on the type. The values tend to be slightly smaller when  $\alpha$  is small and  $\beta$  is large.

**4. Summary discussion.** Several interesting observations can be made concerning the blocks that have been found. The block (5) has played a major role in these investigations, appearing as a maximal trace block for at least some positive  $\alpha$  and  $\beta$  for all four models. Under Model II it is best for all  $\alpha > 0$ , and likewise under Model I, except for small  $\alpha$  combined with small, odd  $p$ . Under Models III and IV, (5) is best for moderate to large  $\alpha$  and  $\beta$

TABLE 3  
String pattern types maximizing (14) for  $\alpha = \beta$ , and Model III efficiencies

$p$	$\alpha$				
	0.1	0.3	0.5	0.7	0.9
3	(2, 2, 1, 0.986)	(2, 2, 1, 0.969)	(1, 3, 0, 0.942)	(1, 3, 0, 0.950)	(1, 3, 0, 0.978)
5	(3, 2, 2, 0.996)	(2, 3, 2, 0.989)	(1, 5, 0, 0.978)	(1, 5, 0, 0.979)	(1, 5, 0, 0.989)
7	(4, 2, 2, 0.998)	(3, 2, 2, 0.996)	(1, 7, 0, 0.988)	(1, 7, 0, 0.988)	(1, 7, 0, 0.993)
9	(5, 2, 2, 0.998)	(3, 4, 2, 0.997)	(1, 9, 0, 0.992)	(1, 9, 0, 0.992)	(1, 9, 0, 0.995)
11	(6, 2, 2, 0.999)	(3, 4, 4, 0.998)	(1, 11, 0, 0.995)	(1, 11, 0, 0.994)	(1, 11, 0, 0.996)
13	(7, 2, 2, 0.999)	(3, 4, 4, 0.999)	(1, 13, 0, 0.996)	(1, 13, 0, 0.996)	(1, 13, 0, 0.997)
15	(8, 2, 2, 0.999)	(4, 4, 4, 0.999)	(2, 8, 7, 0.998)	(1, 15, 0, 0.997)	(1, 15, 0, 0.997)
17	(9, 2, 2, 0.999)	(4, 4, 4, 0.999)	(2, 9, 8, 0.998)	(1, 17, 0, 0.997)	(1, 17, 0, 0.998)
19	(10, 2, 2, 0.999)	(4, 4, 4, 0.999)	(2, 10, 9, 0.999)	(1, 19, 0, 0.998)	(1, 19, 0, 0.998)

combined with small  $p$  growing with the correlations. Since the corresponding design is a BNRC, this says that regardless of inclusion of row or column effects in the model, the two-way correlation pattern, in respecting the row-column layout, has induced requirements akin to those that row and column effects jointly impose. Other BNRC's occur under Models III and IV whenever the string lengths are all even, which is always the case for even  $p$  with Model III. These observations are consistent with what one expects from an examination of the limiting behavior of the information matrices:  $C_d^{(1)} \rightarrow C_d^{(2)}$  and  $C_d^{(3)} \rightarrow C_d^{(4)}$  as  $\alpha \rightarrow 1$ ;  $C_d^{(4)} \rightarrow C_d^{(2)}$  and  $C_d^{(3)} \rightarrow C_d^{(1)}$  as  $\beta \rightarrow 1$ .

Only under Model IV are binary blocks best, and then only for small  $\alpha$  or  $\beta$  in conjunction with small  $p$  which decreases as  $\alpha$  or  $\beta$  increases (Theorem 3.7). This is because only for Model IV is the factor "blocks" the relevant factor for the bottom stratum analysis. In the other models, rows and/or columns are the finer groupings within which the analysis takes place, so it is with respect to those blocking factors that one might expect binarity, at least for small correlations. Thus do Models I and II require binary rows, within the stricture of which they demand the largest possible diagonal neighbor counts. Similarly, for small correlations, Model III demands binary columns (Theorem 3.11) with largest possible diagonal neighbor counts.

As in several of the papers cited in Section 1, all of the designs in this paper have at least  $v(v-1)/2$  blocks, a serious hindrance to their applicability [cf. the comments of Martin and Eccleston (1991), Section 7]. Regardless of this concern with  $b$ , the technical value of the approach is significant, for knowledge of maximal trace blocks will certainly be required at the logical next step: determination of optimal designs which, due to smaller numbers of blocks, cannot enjoy complete symmetry. For positive correlations, the trace maximization problem has been completely solved for Models I and II and has been greatly simplified for Models III and IV by a reduction to the manipulation of pattern types for a single diagonal treatment assignment.

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