

ON THE DETERMINATION OF OPTIMAL DESIGNS FOR AN INTERFERENCE MODEL¹

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This paper generalizes Kushner's method for finding optimal repeated measurements designs to find optimal designs under an interference model. The model we assume is for a one-dimensional layout without guard plots and with different left and right neighbor effects. The resulting optimal designs may need many blocks or may not even exist as a finite design. The results give lower bounds for optimality criteria on finite designs and the design structure can be used to suggest efficient small designs.

1. Introduction. Many agricultural and horticultural trials are susceptible to treatment interference, that is the treatment on one unit affecting the response on neighboring units [see, e.g., Besag and Kempton (1986)]. There is increasing interest in the practical use of models to analyze data from such trials [e.g., David, Monod and Philippeau (1998)] and in the design of experiments in which treatment interference may occur [e.g., David and Kempton (1996)]. A wide variety of possible models have been postulated [e.g., David and Kempton (1996), David, Monod and Philippeau (1998)]. There are only very limited results on optimal designs under interference models. Gill (1993) restricts the class of competing designs to those for which each treatment appears once in each block. Druilhet (1999) avoids this restriction but considers the case of very few blocks. Both papers assume a one-dimensional layout of plots within blocks and that each block has a guard plot at each end, so that each interior plot has two neighbors. They concentrate on model (1) below, or its special case of equal left and right neighbor effects.

The present paper presents a general approach to determine optimal designs for contrasts among direct treatment effects that can be useful for many kinds of interference models. We consider experiments for comparing t treatments using b blocks of size k with a one-dimensional arrangement of plots in each block. We demonstrate the theory for the model with no guard plots and the treatments having different left and right neighbor interference effects. Similar results to the ones given here will be possible for many other related models.

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Let $d(i, j) \in 1, \dots, t$ be the treatment assigned to the plot (i, j) in the j th position of the i th block. In our model the response at plot (i, j) can be written

$$(1) \quad y_{i,j} = \mu + \tau_{d(i,j)} + \lambda_{d(i,j-1)} + \rho_{d(i,j+1)} + \beta_i + e_{i,j}.$$

Here:

- (i) μ is the general mean;
- (ii) $\tau_{d(i,j)}$ is the direct effect of treatment $d(i, j)$;
- (iii) $\lambda_{d(i,j-1)}$ and $\rho_{d(i,j+1)}$ are, respectively, the left and right neighbor effects; that is the interference effect of the treatment assigned to, respectively, the left and right neighbor plots $(i, j - 1)$ and $(i, j + 1)$;
- (iv) β_i is the effect of the i th block; and
- (v) $e_{i,j}$ is the random error, $1 \leq i \leq b, 1 \leq j \leq k$.

We assume that the errors are i.i.d. with expectation 0. The generalization of the method to correlated errors and generalized least squares estimation is straightforward, cf. Kushner (1997). Since we assume there are no guard plots we have $\lambda_{d(i,0)} = \rho_{d(i,k+1)} = 0$.

We seek the optimal design among designs $d \in \Omega_{t,b,k}$, the set of all designs with b blocks of size k and with t treatments. Let T_{du} be the treatment design matrix of the direct effects in block u , $1 \leq u \leq b$. Further define $T_d = [T_{d1}^T, \dots, T_{db}^T]^T$ as the design matrix of direct effects.

Let $Y = [y_{1,1}, \dots, y_{1,k}, y_{2,1}, \dots, y_{b,k}]^T$ be the vector of the observations, 1_k be the k -vector of ones, I_b the b -dimensional identity matrix and \otimes denote the Kronecker product. Let V denote the $k \times k$ left neighbor incidence matrix with (i, j) th element $v_{i,j}$ equal to 1 if $i - j = 1$ and 0 otherwise. For each u we define $L_{du} = VT_{du}$ and $R_{du} = V^T T_{du}$. Then $L_d = [L_{d1}^T, \dots, L_{db}^T]^T = (I_b \otimes V) T_d$ and $R_d = [R_{d1}^T, \dots, R_{db}^T]^T = (I_b \otimes V^T) T_d$ are, respectively, the design matrices of the left and right neighbor effects. Let e be the vector of the errors and let τ, λ, ρ , and β be the vectors of direct effects, of left neighbor effects, of right neighbor effects and of block effects, respectively. Then, we can write model (1) in vector notation as

$$Y = 1_{bk}\mu + T_d\tau + L_d\lambda + R_d\rho + (I_b \otimes 1_k)\beta + e.$$

For an $n \times p$ matrix M define $\omega^\perp(M) = I_n - M(M^T M)^- M^T$, where $(M^T M)^-$ is a generalized inverse (g-inverse) of $M^T M$. Then [see, e.g., Kunert (1983)] the information matrix for the least squares estimate of τ , with zero row and column sums, is

$$C_d = T_d^T \omega^\perp([I_b \otimes 1_k, L_d, R_d]) T_d.$$

A $t \times t$ matrix M is said to be completely symmetric, if all its diagonal elements are equal and all its off-diagonal elements are equal. A completely symmetric information matrix is a scalar multiple of the matrix $B_t = I_t - \frac{1}{t} 1_t 1_t^T$. Assume we have a design $d^* \in \Omega_{t,b,k}$ such that C_{d^*} is completely symmetric and that $\text{tr} C_{d^*}$ is maximal over $\Omega_{t,b,k}$. Then the design d^* is universally optimum, that is, it is optimal under all the optimality criteria considered by Kiefer (1975).

2. Determination of an upper bound for $\text{tr} C_d$. For a partitioned matrix $M = [S, U]$, we can write

$$(2) \quad \omega^\perp([S, U]) = \omega^\perp(S) - \omega^\perp(S)U \{U^T \omega^\perp(S)U\}^- U^T \omega^\perp(S).$$

Applying this formula twice and defining

$$C_{d11} = T_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) T_d, \quad C_{d12} = T_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) L_d, \quad C_{d13} = T_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) R_d, \\ C_{d22} = L_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) L_d, \quad C_{d23} = L_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) R_d, \quad C_{d33} = R_d^T \omega^\perp(I_b \otimes \mathbf{1}_k) R_d$$

we get that

$$(3) \quad C_d = C_{d11} - C_{d12} C_{d22}^- C_{d12}^T - (C_{d13} - C_{d12} C_{d22}^- C_{d23}) \\ \times (C_{d33} - C_{d23}^T C_{d22}^- C_{d23})^- (C_{d13} - C_{d12} C_{d22}^- C_{d23})^T.$$

Note that $\omega^\perp(I_b \otimes \mathbf{1}_k) = I_b \otimes B_k$. The formula for C_d contains g-inverses of C_{d22} and of $C_{d33} - C_{d23}^T C_{d22}^- C_{d23}$, both of which depend on the design d . This makes the determination of $\text{tr} C_d$ for an arbitrary design d difficult. Hence, we try to find a simple upper bound for $\text{tr} C_d$.

The derivation of this bound is inspired by the convexity argument of Pukelsheim [(1993), page 75; see also Kushner (1997), Lemma 5.1]. We give a slightly different proof, which is also valid if the matrices do not have full rank. We begin with a technical proposition.

PROPOSITION 1. *Assume $A_1, \dots, A_n, D_1, \dots, D_n$ are matrices, $A_i \in \mathbb{R}^{m_i \times r}$, $D_i \in \mathbb{R}^{m_i \times s}$, $1 \leq i \leq n$. Then*

$$\sum A_i^T A_i - (\sum A_i^T D_i) (\sum D_i^T D_i)^- (\sum D_i^T A_i) \\ \geq \sum \{A_i^T A_i - A_i^T D_i (D_i^T D_i)^- D_i^T A_i\}$$

in the Loewner-ordering.

PROOF. Consider the partitioned matrices

$$M_1 = \begin{bmatrix} D_1 \\ \vdots \\ D_n \end{bmatrix} \quad \text{and} \quad M_2 = \begin{bmatrix} D_1 & & \\ & \ddots & \\ & & D_n \end{bmatrix}.$$

The column-space of M_1 is contained in the column-space of the block diagonal matrix M_2 . Hence,

$$\omega^\perp(M_1) \geq \omega^\perp(M_2) = \begin{bmatrix} \omega^\perp(D_1) & & \\ & \ddots & \\ & & \omega^\perp(D_n) \end{bmatrix}$$

and

$$\begin{aligned}
& \sum A_i^T A_i - (\sum A_i^T D_i) (\sum D_i^T D_i)^- (\sum D_i^T A_i) \\
&= \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix}^T \omega^\perp(M_1) \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix} \\
&\geq \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix}^T \begin{bmatrix} \omega^\perp(D_1) & & \\ & \ddots & \\ & & \omega^\perp(D_n) \end{bmatrix} \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix} \\
&= \sum (A_i^T A_i - A_i^T D_i (D_i^T D_i)^- D_i^T A_i). \quad \square
\end{aligned}$$

Note that $T_d \mathbf{1}_t$ is in the column-space of $I_b \otimes \mathbf{1}_k$, while $R_d \mathbf{1}_t$ and $L_d \mathbf{1}_t$ are not. This implies [see Kunert (1983)] that C_{d11} has row and column sums zero, that C_{d12} and C_{d13} have column sums zero, but not necessarily row sums zero and that C_{d22} , C_{d23} and C_{d33} need not have zero row sums or column sums. For our bound, we use the traces of $B_t C_{dij} B_t$ and define $c_{dij} = \text{tr} B_t C_{dij} B_t$ for $1 \leq i \leq j \leq 3$.

Since the matrix

$$\begin{bmatrix} B_t C_{d11} B_t & B_t C_{d12} B_t & B_t C_{d13} B_t \\ B_t C_{d12}^T B_t & B_t C_{d22} B_t & B_t C_{d23} B_t \\ B_t C_{d13}^T B_t & B_t C_{d23}^T B_t & B_t C_{d33} B_t \end{bmatrix} = \begin{bmatrix} B_t T_d^T \\ B_t L_d^T \\ B_t R_d^T \end{bmatrix} \omega^\perp(I_b \otimes \mathbf{1}_k) \begin{bmatrix} T_d B_t & L_d B_t & R_d B_t \end{bmatrix}$$

is nonnegative definite, this also holds for

$$\begin{bmatrix} c_{d11} & c_{d12} & c_{d13} \\ c_{d12} & c_{d22} & c_{d23} \\ c_{d13} & c_{d23} & c_{d33} \end{bmatrix}.$$

This implies directly that $c_{dii} \geq 0$, $1 \leq i \leq 3$ and that $c_{d22}c_{d33} - c_{d23}^2 \geq 0$. It also follows that [see, e.g., Rao and Toutenburg (1995), Theorem A74]

$$(4) \quad Q = \begin{bmatrix} c_{d22} & c_{d23} \\ c_{d23} & c_{d33} \end{bmatrix} \text{ satisfies } QQ^- \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix} = \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix},$$

and, consequently, that

$$\begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} Q^- \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix}$$

does not depend on the choice of the g-inverse Q^- .

We are therefore in a position to define

$$q_d^* = c_{d11} - \begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} Q^- \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix}.$$

Then q_d^* depends on the following four cases (i) to (iv):

(i) If $c_{d22}c_{d33} - c_{d23}^2 > 0$, then Q is nonsingular and

$$q_d^* = c_{d11} - \frac{c_{d12}^2 c_{d33} - 2c_{d12}c_{d13}c_{d23} + c_{d13}^2 c_{d22}}{c_{d22}c_{d33} - 2c_{d23}^2}.$$

(ii) If $c_{d22}c_{d33} - c_{d23}^2 = 0$ and $c_{d22} > 0$, then $q_d^* = c_{d11} - c_{d12}^2/c_{d22}$.

(iii) If $c_{d22} = 0$ and $c_{d33} > 0$, then $q_d^* = c_{d11} - c_{d13}^2/c_{d33}$.

(iv) If $c_{d22} = c_{d33} = 0$, then $q_d^* = c_{d11}$.

With these definitions we can show

PROPOSITION 2. *Every design $d \in \Omega_{t,b,k}$ has $\text{tr}C_d \leq q_d^*$. If a design f has all C_{fij} , $1 \leq i \leq j \leq 3$, completely symmetric, then $\text{tr}C_f = q_f^*$.*

PROOF. Using formula (2), C_d can also be written as

$$(5) \quad C_d = \tilde{T}_d^T \omega^\perp([\tilde{L}_d, \tilde{R}_d])\tilde{T}_d,$$

where $\tilde{T}_d = \omega^\perp(I_b \otimes 1_k)T_d$, $\tilde{L}_d = \omega^\perp(I_b \otimes 1_k)L_d$ and $\tilde{R}_d = \omega^\perp(I_b \otimes 1_k)R_d$.

In Proposition 1 let $n = t!$ and consider $\{S_1 = I_t, S_2, \dots, S_n\}$, the set of all $t \times t$ permutation matrices. Then define $A_i = \tilde{T}_d S_i$, $D_i = [\tilde{L}_d S_i, \tilde{R}_d S_i]$, $1 \leq i \leq n$. It can be shown with straightforward algebra, using (3) and (4), that $A_i^T \omega^\perp(D_i) A_i = S_i^T C_d S_i$ for all $1 \leq i \leq n$. On the other hand,

$$\begin{aligned} & \sum A_i^T A_i - (\sum A_i^T D_i) (\sum D_i^T D_i)^- (\sum D_i^T A_i) \\ &= \sum S_i^T \tilde{T}_d^T \tilde{T}_d S_i - \left[\sum S_i^T \tilde{T}_d^T \tilde{L}_d S_i, \sum S_i^T \tilde{T}_d^T \tilde{R}_d S_i \right] \\ & \quad \times \begin{bmatrix} \sum S_i^T \tilde{L}_d^T \tilde{L}_d S_i & \sum S_i^T \tilde{L}_d^T \tilde{R}_d S_i \\ \sum S_i^T \tilde{R}_d^T \tilde{L}_d S_i & \sum S_i^T \tilde{R}_d^T \tilde{R}_d S_i \end{bmatrix}^- \begin{bmatrix} \sum S_i^T \tilde{L}_d^T \tilde{T}_d S_i \\ \sum S_i^T \tilde{R}_d^T \tilde{T}_d S_i \end{bmatrix} \\ &= \sum S_i^T C_{d11} S_i - \left[\sum S_i^T C_{d12} S_i, \sum S_i^T C_{d13} S_i \right] \\ & \quad \times \begin{bmatrix} \sum S_i^T C_{d22} S_i & \sum S_i^T C_{d23} S_i \\ \sum S_i^T C_{d23}^T S_i & \sum S_i^T C_{d33} S_i \end{bmatrix}^- \begin{bmatrix} \sum S_i^T C_{d12}^T S_i \\ \sum S_i^T C_{d13}^T S_i \end{bmatrix}. \end{aligned}$$

Since the summations are over all permutations of the numbers $\{1, \dots, t\}$, we have that $\sum S_i^T C_{drs} S_i$ is completely symmetric for all $1 \leq r \leq s \leq 3$. The fact that C_{d11} , C_{d12} and C_{d13} have column sums zero implies $\sum S_i^T C_{drs} S_i = \{c_{drs}n/(t-1)\}B_t + z_{rs}1_t 1_t^T$ for some z_{rs} , with $z_{rs} = 0$ if $r = 1$. To proceed, we

need a g-inverse of

$$\begin{aligned} F &= \begin{bmatrix} \{c_{d22}n/(t-1)\}B_t + z_{22}\mathbf{1}_t\mathbf{1}_t^T & \{c_{d23}n/(t-1)\}B_t + z_{23}\mathbf{1}_t\mathbf{1}_t^T \\ \{c_{d23}n/(t-1)\}B_t + z_{23}\mathbf{1}_t\mathbf{1}_t^T & \{c_{d33}n/(t-1)\}B_t + z_{33}\mathbf{1}_t\mathbf{1}_t^T \end{bmatrix} \\ &= \frac{n}{t-1}(\mathbf{Q} \otimes B_t) + \begin{bmatrix} z_{22} & z_{23} \\ z_{23} & z_{33} \end{bmatrix} \otimes \mathbf{1}_t\mathbf{1}_t^T. \end{aligned}$$

One such g-inverse, for appropriate w_{ij} , is

$$F^- = \frac{t-1}{n} \left(\mathbf{Q}^- \otimes B_t - \begin{bmatrix} w_{22} & w_{23} \\ w_{23} & w_{33} \end{bmatrix} \otimes \mathbf{1}_t\mathbf{1}_t^T \right).$$

Therefore

$$\begin{aligned} &\sum A_i^T A_i - (\sum A_i^T D_i) (\sum D_i^T D_i)^- (\sum D_i^T A_i) \\ &= \frac{n}{t-1} c_{d11} B_t - \frac{n^2}{(t-1)^2} ([c_{d12}, c_{d13}] \otimes B_t) F^- \left(\begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix} \otimes B_t \right) \\ &= \frac{n}{t-1} q_d^* B_t. \end{aligned}$$

Then Proposition 1 implies that $\text{tr}C_d \leq q_d^*$.

Finally note that for design f we have $C_{frs} = \sum S_i^T C_{frs} S_i / n$ for every $1 \leq r \leq s \leq 3$. \square

3. Methods for determination of a maximal q_d^* . An optimal design d^* should have a completely symmetric C_{d^*} , with $\text{tr}C_{d^*} = q_d^*$ and it should have the right proportions of blocks assigned to the treatment sequences such that q_d^* is maximal. Therefore, we need to maximize the bound q_d^* . Define

$$\begin{aligned} c_{d11}^{(u)} &= \text{tr}(T_{du}^T B_k T_{du}), & c_{d12}^{(u)} &= \text{tr}(T_{du}^T B_k L_{du}), & c_{d13}^{(u)} &= \text{tr}(T_{du}^T B_k R_{du}), \\ c_{d22}^{(u)} &= \text{tr}(B_t L_{du}^T B_k L_{du} B_t), & c_{d23}^{(u)} &= \text{tr}(B_t L_{du}^T B_k R_{du} B_t) \quad \text{and} \\ c_{d33}^{(u)} &= \text{tr}(B_t R_{du}^T B_k R_{du} B_t). \end{aligned}$$

We then get that

$$c_{drs} = \sum_{u=1}^b c_{drs}^{(u)}, \quad 1 \leq r \leq s \leq 3.$$

Note that each $c_{drs}^{(u)}$ remains unchanged if the treatments are relabelled, i.e. if T_{du} , L_{du} and R_{du} are replaced by $T_{du}S$, $L_{du}S$ and $R_{du}S$, respectively, where S is any $t \times t$ permutation matrix. We call two sequences of treatments equivalent if one can be transformed to the other by relabelling the treatments. Hence, two equivalent treatment sequences give the same $c_{drs}^{(u)}$. Therefore, for given t and k , we can divide the set of all possible treatment sequences into K equivalence classes s_1, \dots, s_K . If, for example, $k = 3$ and $t \geq 3$, then there are the $K = 5$ equivalence classes given in Table 1.

Since $c_{drs}^{(u)}$ is the same for each u receiving a treatment sequence in a given equivalence class s_ℓ , $1 \leq \ell \leq K$, we can define $c_{rs}(\ell) = c_{drs}^{(u)}$ and get $c_{drs} = b \sum_{\ell=1}^K \pi_{d\ell} c_{rs}(\ell)$, where $\pi_{d\ell}$ is the proportion of blocks assigned to the class s_ℓ . This, however, implies that the bound q_d^* of any design $d \in \Omega_{t,b,k}$ is determined by the proportions $\pi_{d\ell}$. Note that the c_{dij} are linear in the $\pi_{d\ell}$, but that q_d^* is a quotient, where the $\pi_{d\ell}$ are third order in the numerator and second order in the denominator. This makes the maximization of q_d^* difficult.

The situation is similar to the models (with carryover effects) for repeated measurements designs. For these Kushner (1997) showed how to use the linearity of the c_{drs} to maximize q_d^* . This idea can be generalized to interference models.

PROPOSITION 3. *For any design $d \in \Omega_{t,b,k}$ define the function $q_d : \mathbb{R}^2 \rightarrow \mathbb{R}$ as*

$$q_d(x, y) = c_{d11} + 2c_{d12}x + 2c_{d13}y + 2c_{d23}xy + c_{d22}x^2 + c_{d33}y^2.$$

Then for every x and y , we have $q_d(x, y) \geq q_d^$. There is at least one point (x_d, y_d) such that $q_d(x_d, y_d) = q_d^*$.*

PROOF. We can write

$$\begin{aligned} q_d(x, y) &= c_{d11} + 2 \begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} x & y \end{bmatrix} \mathbf{Q} \begin{bmatrix} x \\ y \end{bmatrix} \\ &= c_{d11} + 2 \begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} \left(u - \mathbf{Q}^{-1} \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix} \right) \\ &\quad + (u^T - \begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} \mathbf{Q}^{-1}) \mathbf{Q} \left(u - \mathbf{Q}^{-1} \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix} \right) \end{aligned}$$

where

$$u = \begin{bmatrix} x \\ y \end{bmatrix} + \mathbf{Q}^{-1} \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix}.$$

Then equation (4) implies that

$$q_d(x, y) = c_{d11} - \begin{bmatrix} c_{d12} & c_{d13} \end{bmatrix} \mathbf{Q}^{-1} \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix} + u^T \mathbf{Q} u.$$

Therefore, $q_d(x, y)$ is minimal iff $\mathbf{Q}u = 0$, that is, iff

$$\mathbf{Q} \begin{bmatrix} x \\ y \end{bmatrix} = - \begin{bmatrix} c_{d12} \\ c_{d13} \end{bmatrix}.$$

This, however, holds if and only if the partial derivatives of q_d with respect to x and y are both 0. The minimum of q_d equals q_d^* . \square

From the proof of Proposition 3, we immediately get the following corollary:

COROLLARY 1. Consider a point (x_d, y_d) such that the partial derivatives $\partial q_d(x, y)/\partial x$ and $\partial q_d(x, y)/\partial y$ are both 0 for $(x, y) = (x_d, y_d)$. Then $q_d(x_d, y_d) = q_d^*$.

The elegance of $q_d(x, y)$ is that it can be written as a linear combination of functions $h_\ell(x, y)$, which depend on the equivalence classes of treatment sequences. Define

$$h_\ell(x, y) = c_{11}(\ell) + 2c_{12}(\ell)x + 2c_{13}(\ell)y + 2c_{23}(\ell)xy + c_{22}(\ell)x^2 + c_{33}(\ell)y^2,$$

for every $1 \leq \ell \leq K$. Then

$$q_d(x, y) = b \sum_{\ell=1}^K \pi_{d\ell} h_\ell(x, y).$$

PROPOSITION 4. For a design $d \in \Omega_{t,b,k}$ consider a point (x_d, y_d) for which $q_d(x_d, y_d) = q_d^*$. If $b h_\ell(x_d, y_d) \leq q_d(x_d, y_d) = q_d^*$ for every $1 \leq \ell \leq K$, then for every $f \in \Omega_{t,b,k}$ we have $\text{tr}C_f \leq q_d^* = \alpha_{t,b,k}^*$, say.

PROOF. For any f we have

$$q_f^* = b \sum_{\ell=1}^K \pi_{f\ell} h_\ell(x_f, y_f) \leq \sum_{\ell=1}^K \pi_{f\ell} b h_\ell(x_d, y_d) \leq \sum_{\ell=1}^K \pi_{f\ell} q_d^* = q_d^*.$$

The rest follows from Proposition 2. \square

Note that the proportions $\pi_{d\ell}$ must be such that the partial derivatives of $\sum \pi_{d\ell} h_\ell(x, y)$ at (x_d, y_d) are both 0 and that only such classes ℓ of sequences are included for which $h_\ell(x_d, y_d) = \max_{1 \leq \ell \leq K} h_\ell(x_d, y_d)$. Therefore (x_d, y_d) must be either at the minimum of an h_ℓ or at the intersection of two or more of the h_ℓ .

In many situations there is no design fulfilling both the conditions of Proposition 4 and of Proposition 2. In that case, however, one practical use of the $\alpha_{t,b,k}^*$ is the lower bound which it provides for the optimality criteria.

As an example, consider the A-criterion $\varphi_A(C_f)$, which is the trace of the Moore-Penrose generalized inverse of C_f . From Proposition 2 we get

$$\varphi_A(C_f) \geq \varphi_A \left(\frac{q_f^*}{t-1} B_t \right) = \text{tr} \left(\frac{t-1}{q_f^*} B_t \right) = \frac{(t-1)^2}{q_f^*}.$$

With Proposition 4 it follows that

$$\varphi_A(C_f) \geq \frac{(t-1)^2}{\alpha_{t,b,k}^*}.$$

4. Some examples. In this section we demonstrate the methods derived in this paper by finding optimal or efficient designs for $k = 3$ and 4 for all $t \geq 2$. Note that, to save space, blocks are represented as columns in Examples 1 to 4.

4.1. *The case of 3 plots per block.* Table 1 lists the equivalence classes and the corresponding $c_{rs}(\ell)$ for the case that there are $k = 3$ plots per block. If $t = 2$, then only the first four sequences are possible.

A design d^* which has half of its sequences from s_2 and half of its sequences from s_4 has

$$q_{d^*}(x, y) = b \left\{ \frac{1}{2}h_2(x, y) + \frac{1}{2}h_4(x, y) \right\} \\ = b \left(\frac{4}{3} - \frac{1}{3}x - \frac{1}{3}y - \frac{4t-2}{3t}xy + \frac{3t-2}{3t}x^2 + \frac{3t-2}{3t}y^2 \right).$$

If $x = y = t/\{2(t-1)\}$, then the derivatives of $q_{d^*}(x, y)$ with respect to x and y are both 0. Therefore from Corollary 1, we have

$$x_{d^*} = y_{d^*} = \frac{t}{2(t-1)} \quad \text{and} \quad q_{d^*}^* = q_{d^*}(x_{d^*}, y_{d^*}) = \left(\frac{7t-8}{6(t-1)} \right) b.$$

To prove the optimality of $q_{d^*}^*$ we have to calculate $h_\ell(x_{d^*}, y_{d^*})$ for every $1 \leq \ell \leq 5$, and to verify that $q_{d^*}^*/b - h_\ell(x_{d^*}, y_{d^*})$ is nonnegative for every ℓ . Some algebra shows that $q_{d^*}^*/b - h_\ell(x_{d^*}, y_{d^*})$ equals $(3t-4)/(4t-4) > 0$, 0 , $(3t^2-5t)/(3t^2-6t+3) > 0$, 0 , $(t-2)/(3t^2-6t+3) > 0$ (since $t > 2$) for $\ell = 1, \dots, 5$, respectively.

Hence, we have shown:

THEOREM 1. *If $k = 3$ and $t \geq 2$, then for any design $d \in \Omega_{t,b,3}$ we have*

$$trC_d \leq \alpha_{t,b,3}^* = \left(\frac{7t-8}{6(t-1)} \right) b.$$

If a design d^ has half of its blocks with treatment sequences which are equivalent to [1 1 2] and half of its blocks with treatment sequences equivalent to [1 2 2] and if $C_{d^*11}, C_{d^*12}, C_{d^*13}, C_{d^*22}, C_{d^*23}$, and C_{d^*33} are completely symmetric, then d^* is universally optimal over $\Omega_{t,b,3}$.*

TABLE 1
The classes s_ℓ of sequences and adjusted $c_{rs}(\ell)$ for $k = 3, t \geq 2$

ℓ	Representative sequence	$3c_{11}(\ell)$	$3c_{12}(\ell)$	$3c_{13}(\ell)$	$3c_{22}(\ell) + \frac{2}{t}$	$3c_{23}(\ell) - \frac{1}{t}$	$3c_{33}(\ell) + \frac{2}{t}$
1	[1 1 1]	0	0	0	2	-1	2
2	[1 1 2]	4	-1	0	2	-2	4
3	[1 2 1]	4	-3	-3	4	1	4
4	[1 2 2]	4	0	-1	4	-2	2
5	[1 2 3]	6	-2	-2	4	-1	4

EXAMPLE 1. If $t = 2$, then a 4 block example of a design fulfilling the conditions of Theorem 1 is

$$d_1^* = \begin{bmatrix} 1 & 2 & 1 & 2 \\ 1 & 2 & 2 & 1 \\ 2 & 1 & 2 & 1 \end{bmatrix} \in \Omega_{2,4,3}.$$

If $t = 3$ then a 12 block example of a design fulfilling the conditions of Theorem 1 is

$$d_2^* = \begin{bmatrix} 1 & 1 & 2 & 2 & 3 & 3 & 1 & 1 & 2 & 2 & 3 & 3 \\ 1 & 1 & 2 & 2 & 3 & 3 & 2 & 3 & 1 & 3 & 1 & 2 \\ 2 & 3 & 1 & 3 & 1 & 2 & 2 & 3 & 1 & 3 & 1 & 2 \end{bmatrix} \in \Omega_{3,12,3}.$$

If $t = 4$, then a 24 block example is

$$d_3^* = \begin{bmatrix} 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 4 & 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 4 \\ 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 4 & 2 & 3 & 4 & 1 & 3 & 4 & 1 & 2 & 4 & 1 & 2 & 3 \\ 2 & 3 & 4 & 1 & 3 & 4 & 1 & 2 & 4 & 1 & 2 & 3 & 2 & 3 & 4 & 1 & 3 & 4 & 1 & 2 & 4 & 1 & 2 & 3 \end{bmatrix} \in \Omega_{4,24,3}.$$

4.2. *The case of 4 plots per block.* If $k = 4$ and $t \geq 4$, then we have 15 equivalence classes. The representative sequences and the $c_{rs}(\ell)$ for the 15 classes are given in Table 2. For $t = 3$, only the 14 classes s_1 to s_{14} are possible. For $t = 2$, only the 8 classes $s_1, s_2, s_3, s_4, s_6, s_7, s_9$ and s_{10} are possible.

We start with the case $t = 2$. Then consider a design d^* with half of its blocks from s_4 and half of its blocks from s_9 . In that case

$$q_{d^*}(x, y) = b\left\{\frac{1}{2}h_4(x, y) + \frac{1}{2}h_9(x, y)\right\} = b\left(2 + \frac{11}{8}x^2 - 2xy + \frac{11}{8}y^2\right) \geq 2b,$$

with equality holding iff $x = y = 0$. Now, $h_\ell(0, 0) = c_{11}(\ell) \leq 2$ for all 8 possible classes s_ℓ of sequences, with equality for $\ell = 4, 7$ and 9 . Thus we have shown

THEOREM 2. *If $t = 2$ and $k = 4$, then for every design $d \in \Omega_{2,b,4}$ we have $\text{tr}C_d \leq a_{2,b,4}^* = 2b$. If a design d^* has $b/4$ of its blocks with each of the sequences $[1 \ 1 \ 2 \ 2]$, $[2 \ 2 \ 1 \ 1]$, $[1 \ 2 \ 2 \ 1]$ and $[2 \ 1 \ 1 \ 2]$, then d^* is universally optimal over $\Omega_{2,b,4}$.*

Note that sequences $[1 \ 1 \ 2 \ 2]$ and $[2 \ 2 \ 1 \ 1]$ are from s_4 , while $[1 \ 2 \ 2 \ 1]$ and $[2 \ 1 \ 1 \ 2]$ are from s_9 . Because $h_7(0, 0) = 2$, it is possible to show that there is another design f that has $q_f^* = a_{2,b,k}^*$. Design f has $3b/4$ of its blocks with sequences from s_4 and $b/4$ with sequences from s_7 .

TABLE 2
The classes s_ℓ of sequences and adjusted $c_{rs}(\ell)$ for $k = 4$

ℓ	Representative sequence	$4c_{11}(\ell)$	$4c_{12}(\ell)$	$4c_{13}(\ell)$	$4c_{22}(\ell) + \frac{3}{t}$	$4c_{23}(\ell) - \frac{1}{t}$	$4c_{33}(\ell) + \frac{3}{t}$
1	[1 1 1 1]	0	0	0	3	-1	3
2	[1 1 1 2]	6	-1	1	3	-2	7
3	[1 1 2 1]	6	-3	-3	7	-1	7
4	[1 1 2 2]	8	2	2	7	-4	7
5	[1 1 2 3]	10	-1	0	7	-3	9
6	[1 2 1 1]	6	-3	-3	7	-1	7
7	[1 2 1 2]	8	-6	-6	7	4	7
8	[1 2 1 3]	10	-5	-4	7	1	9
9	[1 2 2 1]	8	-2	-2	7	-5	7
10	[1 2 2 2]	6	1	-1	7	-2	3
11	[1 2 2 3]	10	-1	-1	7	-4	7
12	[1 2 3 1]	10	-4	-4	9	-3	9
13	[1 2 3 2]	10	-4	-5	9	1	7
14	[1 2 3 3]	10	0	-1	9	-3	7
15	[1 2 3 4]	12	-3	-3	9	-2	9

EXAMPLE 2. Theorem 2 requires that b is divisible by 4. Suppose $b = 2$ and consider the two designs

$$d = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 2 & 2 \\ 2 & 1 \end{bmatrix} \quad \text{and} \quad f = \begin{bmatrix} 1 & 2 \\ 1 & 1 \\ 2 & 2 \\ 2 & 1 \end{bmatrix}.$$

While $q_d^* = a_{2,2,4}^* = 4$, for d we have $\text{tr}C_d = 16/7 < 4$, because C_{d33} is not completely symmetric. Design f , for which the C_{dij} , except for C_{d23} , are completely symmetric, has $\text{tr}C_d = 3$. Calculating the information matrix for all 256 possible designs, we find that f is universally optimal (since $\text{rank}C_d = 1$).

As $h_{14}(0, 0) = c_{11}(14) = 10/4 > 2$, an optimal design for $t = 3$ must have other sequences than just s_4 , s_7 and s_9 . The case $k = 3$ suggests the candidate design d^* with $\pi_{d^*5} = \pi_{d^*14} = \frac{1}{2}$. In fact, we find that $q_{d^*}(x, y) = b(\frac{5}{2} - \frac{1}{4}x - \frac{1}{4}y - \frac{4}{3}xy + \frac{7}{4}x^2 + \frac{7}{4}y^2)$, with a minimum at $x_{d^*} = y_{d^*} = 3/26$. Therefore $q_{d^*}^* = q_{d^*}(x_{d^*}, y_{d^*}) = (257/104)b$. It is easy to check that for every ℓ , $1 \leq \ell \leq 14$, we have $257/104 - h_\ell(x_{d^*}, y_{d^*}) \geq 0$, with equality holding only for $\ell = 5$ and $\ell = 14$. Hence, we have shown:

THEOREM 3. If $k = 4$ and $t = 3$, then for any design $d \in \Omega_{3,b,4}$ we have $\text{tr}C_d \leq a_{3,b,4}^* = (257/104)b$. If a design d^* has $b/2$ blocks with treatment sequences which are equivalent to each of [1 1 2 3] and [1 2 3 3], and if

C_{d^*11} , C_{d^*12} , C_{d^*13} , C_{d^*22} , C_{d^*23} and C_{d^*33} are completely symmetric, then d^* is universally optimal over $\Omega_{3,b,4}$.

EXAMPLE 3. The design

$$d^* = \begin{bmatrix} 1 & 2 & 3 & 3 & 1 & 2 & 1 & 2 & 3 & 2 & 3 & 1 \\ 1 & 2 & 3 & 2 & 3 & 1 & 1 & 2 & 3 & 3 & 1 & 2 \\ 2 & 3 & 1 & 1 & 2 & 3 & 3 & 1 & 2 & 1 & 2 & 3 \\ 3 & 1 & 2 & 1 & 2 & 3 & 2 & 3 & 1 & 1 & 2 & 3 \end{bmatrix} \in \Omega_{3,12,4}$$

fulfills the conditions of Theorem 3. The first 6 blocks of d^* form a design d which maximizes q_d^* in $\Omega_{3,6,4}$ but for which $\text{tr}C_d < q_d^*$, since C_{d12} and C_{d13} are not completely symmetric. However, when we calculate the A-criterion $\varphi_A(C_d)$ of d and compare it to the unattainable lower bound $\varphi_A^* = (t-1)^2/a_{3,b,4}^*$, then we find that $\varphi_A^*/\varphi_A(C_d) = 0.996$; that is, d has an efficiency of 99.6% and is likely to be A-optimal.

Finally, we consider the case $k = 4$ and $t \geq 4$. We try a design with a proportion π of sequences from the class s_{15} and proportions $(1-\pi)/2$ of classes s_5 and s_{14} , each. The three $h_\ell(x, y)$ intersect at $x = y = (5 - \sqrt{17})/4 = x^*$, say. For $x = y = x^*$, we have

$$h_5(x, y) = h_{14}(x, y) = h_{15}(x, y) = \frac{(135 - 23\sqrt{17})t - (42 - 10\sqrt{17})}{16t}.$$

Note that $h_{15}(x, y) = h_{15}(y, x)$. Thus the derivative of $h_{15}(x + \delta, x - \delta)$ with respect to δ is zero if $\delta = 0$. The same holds for $\frac{1}{2}h_5(x, y) + \frac{1}{2}h_{14}(x, y)$. It hence remains to find a π such that

$$\frac{\partial}{\partial x} \left(\pi h_{15}(x, x) - \frac{1-\pi}{2} h_5(x, x) + \frac{1-\pi}{2} h_{14}(x, x) \right)$$

is zero for $x = x^* \approx 0.219$. Therefore, set

$$\pi = \frac{(23 - 5\sqrt{17})t - (10 - 2\sqrt{17})}{2\sqrt{17}t} = \pi^* \quad \text{say.}$$

It is easy to see that the differences $h_5(x^*, x^*) - h_\ell(x^*, x^*)$, for $\ell = 1, 2, \dots, 15$ are all positive, except for $\ell = 4, 5, 14$ and 15 , when they are 0.

Hence we have an optimal design using sequence classes s_5 , s_{14} and s_{15} . Since $h_5(x^*, x^*) - h_4(x^*, x^*) = 0$, we can construct an optimal design with some sequences from the class s_4 . In fact, a second optimal design exists which consists of s_4 and s_{15} only having a proportion

$$\delta^* = \frac{(23 - 3\sqrt{17})t - (10 - 2\sqrt{17})}{4\sqrt{17}t}$$

of sequences from the class s_{15} and a proportion of $1 - \delta^*$ of sequences from s_4 . Any convex combination of these two designs is also optimal. Hence, we have shown:

THEOREM 4. *If $k = 4$ and $t \geq 4$, then for every design $d \in \Omega_{t,b,4}$ we have*

$$\text{tr}C_d \leq \alpha_{t,b,4}^* = b \frac{(135 - 23\sqrt{17})t - (42 - 10\sqrt{17})}{16t}.$$

To achieve this bound, we would need to construct a design d^* as follows:

Define

$$\pi^* = \frac{(23 - 5\sqrt{17})t - (10 - 2\sqrt{17})}{2\sqrt{17}t} \quad \text{and} \quad \delta^* = \frac{(23 - 3\sqrt{17})t - (10 - 2\sqrt{17})}{4\sqrt{17}t}.$$

Choose $0 \leq \alpha \leq 1$. Let proportions $(1 - \alpha)(1 - \delta^*)$, $\alpha(1 - \pi^*)/2$, $\alpha(1 - \pi^*)/2$ and $(\alpha\pi^* + (1 - \alpha)\delta^*)$ of the blocks of d^* have treatment sequences which are equivalent to $[1\ 1\ 2\ 2]$, $[1\ 1\ 2\ 3]$, $[1\ 2\ 3\ 3]$ and $[1\ 2\ 3\ 4]$, respectively, such that C_{d^*11} , C_{d^*12} , C_{d^*13} , C_{d^*22} , C_{d^*23} and C_{d^*33} are completely symmetric.

REMARK. The design d^* in Theorem 4 cannot exist for finite b . To see this, note that $1 - \delta^* = (1 - \pi^*)/2$, which is irrational. Therefore, $(1 - \alpha)(1 - \delta^*) = (1 - \alpha)(1 - \pi^*)/2$ and there is no α such that both $(1 - \alpha)(1 - \pi^*)/2$ and $\alpha(1 - \pi^*)/2$ are rational.

Despite the non-existence of d^* , Theorem 4 has two useful aspects. First, it suggests the structure of an efficient design, and second, $\alpha_{v,b,4}^*$ gives a lower bound for the A-value. This is demonstrated in Example 4.

EXAMPLE 4. It is possible to construct highly efficient designs if we can approximate reasonably well the fractions π^* or δ^* from Theorem 4. If $t = 4$, then the upper bound $\alpha_{4,b,4}^*$ for $\text{tr}C_d$ is approximately $b \times 2.49852$. To construct an efficient design, we select $\alpha = 0$. We would need a proportion of $\delta^* \approx 0.617995$ of blocks with a sequence from s_{15} . We use $2/3$ instead and construct the 36 block design

$$f = \begin{bmatrix} 1\ 1\ 1\ 2\ 2\ 2\ 3\ 3\ 3\ 4\ 4\ 4\ 1\ 2\ 3\ 4\ 1\ 2\ 4\ 3\ 1\ 4\ 3\ 2\ 1\ 2\ 3\ 4\ 1\ 2\ 4\ 3\ 1\ 4\ 3\ 2 \\ 1\ 1\ 1\ 2\ 2\ 2\ 3\ 3\ 3\ 4\ 4\ 4\ 2\ 4\ 1\ 3\ 2\ 3\ 1\ 4\ 4\ 2\ 1\ 3\ 2\ 4\ 1\ 3\ 2\ 3\ 1\ 4\ 4\ 2\ 1\ 3 \\ 2\ 3\ 4\ 1\ 3\ 4\ 1\ 2\ 4\ 1\ 2\ 3\ 3\ 1\ 4\ 2\ 4\ 1\ 3\ 2\ 3\ 1\ 2\ 4\ 3\ 1\ 4\ 2\ 4\ 1\ 3\ 2\ 3\ 1\ 2\ 4 \\ 2\ 3\ 4\ 1\ 3\ 4\ 1\ 2\ 4\ 1\ 2\ 3\ 4\ 3\ 2\ 1\ 3\ 4\ 2\ 1\ 2\ 3\ 4\ 1\ 4\ 3\ 2\ 1\ 3\ 4\ 2\ 1\ 2\ 3\ 4\ 1 \end{bmatrix} \in \Omega_{4,36,4}.$$

It is easy to verify that C_{f11}, \dots, C_{f33} are completely symmetric and that $\text{tr}C_f \approx 89.8064$. This is extremely close to the upper bound which is approximately $36 \times 2.49852 = 89.94672$, so that f is highly efficient (efficiency ≈ 0.9984).

With 12 blocks, a design similarly constituted to f is

$$g_1 = \begin{bmatrix} 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 4 & 3 \\ 1 & 2 & 3 & 4 & 2 & 4 & 1 & 3 & 2 & 3 & 1 & 4 \\ 2 & 3 & 4 & 1 & 3 & 1 & 4 & 2 & 4 & 1 & 3 & 2 \\ 2 & 3 & 4 & 1 & 4 & 3 & 2 & 1 & 3 & 4 & 2 & 1 \end{bmatrix} \in \Omega_{4,12,4}.$$

Its C_g is not completely symmetric. However, its relative A-efficiency with respect to the bound $(t-1)^2/a_{4,12,4}^*$ is 0.968.

If we prefer not to repeat treatments, we have the universally optimal binary design using a type I orthogonal array with efficiency 0.924:

$$h = \begin{bmatrix} 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\ 3 & 1 & 4 & 2 & 2 & 4 & 1 & 3 & 2 & 3 & 4 & 1 \\ 2 & 4 & 1 & 3 & 3 & 1 & 4 & 2 & 4 & 1 & 2 & 3 \\ 4 & 3 & 2 & 1 & 4 & 3 & 2 & 1 & 3 & 4 & 1 & 2 \end{bmatrix}.$$

With 6 blocks, a design with relative A-efficiency 0.885, similarly constituted to f is

$$g_2 = \begin{bmatrix} 1 & 3 & 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 4 & 1 & 3 \\ 2 & 4 & 3 & 1 & 4 & 2 \\ 2 & 4 & 4 & 3 & 2 & 1 \end{bmatrix} \in \Omega_{4,6,4}.$$

For 8 treatments and 24 blocks, similar ideas lead to the design $g_3 \in \Omega_{8,24,4}$, where

$$g_3 = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 1 & 1 & 3 & 6 & 2 & 2 & 6 & 5 & 4 & 7 & 8 & 8 & 3 & 5 & 4 & 7 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 2 & 4 & 1 & 7 & 5 & 8 & 3 & 6 & 3 & 2 & 6 & 1 & 8 & 7 & 5 & 4 \\ 5 & 6 & 7 & 8 & 1 & 2 & 3 & 4 & 3 & 2 & 6 & 1 & 8 & 7 & 5 & 4 & 2 & 4 & 1 & 7 & 5 & 8 & 3 & 6 \\ 5 & 6 & 7 & 8 & 1 & 2 & 3 & 4 & 4 & 7 & 8 & 8 & 3 & 5 & 4 & 7 & 1 & 1 & 3 & 6 & 2 & 2 & 6 & 5 \end{bmatrix}.$$

This design has a relative A-efficiency of 0.910. Note that each treatment is replicated 12 times in the design g_3 , as in g_1 .

The methods of the present paper can be used for blocks with $k > 4$ as well. However, with larger k the number K of equivalence classes increases rapidly. For $k = 5$ and $t = 5$ there are 52 classes of sequences. It is possible, though, to show that a design d with a proportion

$$\pi^* = \frac{3}{4\sqrt{41t}} \left(25t - 3\sqrt{41t} - 7 + \sqrt{41} \right)$$

of blocks with a sequence equivalent to $[1 \ 2 \ 3 \ 4 \ 5]$ and the other blocks with a sequence equivalent to $[1 \ 1 \ 2 \ 3 \ 3]$ has a maximal $q_d^* = a_{t,b,5}^*$. In the special

instance $t = 5$ (with $\pi^* \approx 0.6643$), then a binary type I orthogonal array h , which uses only sequences equivalent to $[1\ 2\ 3\ 4\ 5]$, has an efficiency of $q_h^*/a_{5,b,5}^* = 0.959$. This is slightly higher than for $k = 4$.

Further work is aimed at obtaining bounds on the $c_{ij}(\ell)$ to get results for a general k . We conjecture that $a_{t,b,k}^*$ is achieved by a design with a majority of sequences from the class containing $[1\ 2\ 3 \dots k-2\ k-1\ k]$ and the rest of the sequences equivalent to $[1\ 1\ 2 \dots k-3\ k-2\ k-2]$. We also conjecture that for $t \geq k > 5$, a binary type I orthogonal array will have an efficiency of more than 0.95.

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