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Optimal designs for an interference model

Joachim Kunert, Sabine Mersmann

Technische Universität Dortmund

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Sonderforschungsbereich 475
Universität Dortmund
44221 Dortmund
Germany

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Joachim Kunert and Sabine Mersmann*

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Abstract

Kunert and Martin (2000) determined optimal and efficient block designs in a model for field trials with interference effects, for block sizes up to 4. In this paper we use Kushner's method (Kushner, 1997) of finding optimal approximate designs to extend the work of Kunert and Martin (2000) to optimal designs with five or more plots per block. We give an overall upper bound $a^*_{t,b,k}$ for the trace of the information matrix of any design and show that an universally optimal approximate design will have all its sequences from merely four different equivalence classes. We further determine the efficiency of a binary type I orthogonal array under the general Φ_p-criterion. We find that these designs achieve high efficiencies of more than 0.94.

1 Introduction

The possibility of interference effects is a concern in agricultural field trials. A number of papers demonstrate the presence of such effects in agricultural experiments, see e.g. Clarke et al. (2000), David et al. (2001) or Connolly et al. (2008). Various models and experimental designs have been proposed to cope with interference effects, see e.g. Kempton (1982), Kunert and Martin (2000), Filipiak and Markiewicz (2003, 2005), and Bailey and Druilhet (2004). The present paper extends the results of Kunert and Martin (2000) on universal optimality in a model with possibly different interference effects from two sides.

Kiefer (1975) introduced the concept of universal optimality, which covers many well-known optimality criteria, such as the A-criterion or the D-criterion. Nevertheless, in models with interference effects it remains difficult to determine optimal or even sufficiently efficient designs. Using a method originally described by Kushner (1997), Kunert and Martin (2000) determined universally optimal designs for a block model assuming different left and right neighbour effects in the case of blocks of size 3. For blocks of size 4, they found highly efficient designs. Additionally, they conjectured

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that designs constructed from certain classes of sequences should be efficient, possibly optimal, for blocks of size 5 or larger.

In this paper we use Kushner's method (Kushner, 1997) to further investigate the conjecture of Kunert and Martin (2000) about optimal designs with five or more plots per block. In section 2 we describe our statistical model and introduce some notation. In section 3 we give an upper bound for the trace of the information matrix and show how an universally optimal approximate design should be structured for an arbitrary number k of plots per block and $t \geq k$ treatments. In particular, we determine good classes of treatment sequences and the proportions in which they should be used in an optimal design.

In section 4, we derive a formula for the efficiency of an orthogonal array of type I $OA_I(b,k,t,2)$. An $OA_I(b,k,t,2)$ is an arrangement of t symbols into b rows and k columns, such that the rows of every two columns contain all $(t-1)t$ pairs of distinct symbols equally often. See Rao (1961) for more details. We show that for any t and b the efficiency of an $OA_I(b,k,t,2)$ is at least 0.94 under any Φ_p-criterion.

2 Model and notation

We assume an experimental field with b blocks of size k and t treatments. A design for such an experiment is a mapping $d : \{1,\ldots,b\} \times \{1,\ldots k\} \rightarrow \{1,\ldots t\}$ that assigns treatment $d(i,\,j)$ to plot $(i,\,j)$ of the field. The set of all possible designs d for such an experiment is denoted by $\Omega_{t,b,k}$.

In this paper we consider an interference model with different left and right neighbour effects, as in Kunert and Martin (2000). Thus, the observation y_{ij} at plot $(i,\,j)$, $1 \leq i \leq b$, $1 \leq j \leq k$ is modelled as

$$y_{ij} = \mu + \beta_i + \tau_{d(i,\,j)} + \lambda_{d(i,\,j-1)} + \rho_{d(i,\,j+1)} + e_{ij}, \tag{2.1}$$

where μ denotes the general mean, β_i is the effect of the i-th block, $\tau_{d(i,j)}$ the direct effect of the treatment applied to plot (i,j), $\lambda_{d(i,j-1)}$ and $\rho_{d(i,j+1)}$ are left and right neighbour effects, respectively and e_{ij} is the random error. Like Kunert and Martin (2000) we postulate that there are no guard plots, so that $\lambda_{d(i,0)} = \rho_{d(i,k+1)} = 0$ for all $i = 1,\ldots,b$.

Every design $d \in \Omega_{t,b,k}$ consists of b treatment sequences $s_1(d),\ldots,s_b(d)$, where $s_i(d)$ indicates the sequence of treatments applied to the i-th block. Let V denote the $k \times k$ matrix with elements $V(i,j) = 1$ if $i - j = 1$ and 0 otherwise. We denote by T_s the design matrix of direct effects in a block receiving sequence s and define $L_s = VT_s$ and $R_s = V^T T_s$. Then model (2.1) in matrix notation becomes

$$Y = 1_{bk}\mu + (I_b \otimes 1_k)\beta + T_d\tau + L_d\lambda + R_d\rho + e, \tag{2.2}$$

where $Y = (y_{11}, \ldots, y_{1k}, \ldots, y_{b1}, \ldots, y_{bk})^T \in \mathbb{R}^{bk}$ is the vector of observations, $1_{bk} \in \mathbb{R}^{bk}$ denotes the bk-vector of ones and $I_b \otimes 1_k \in \mathbb{R}^{bk \times b}$ is the design matrix of block effects, where $\otimes$ stands for the Kronecker product and I_b denotes the $b \times b$ identity matrix. Further, $T_d = (T^T_{s_1(d)}, \ldots, T^T_{s_b(d)})^T \in \mathbb{R}^{bk \times t}$ is the design matrix of direct effects, and $L_d = (L^T_{s_1(d)}, \ldots, L^T_{s_b(d)})^T \in \mathbb{R}^{bk \times t}$ and $R_d = (R^T_{s_1(d)}, \ldots, R^T_{s_b(d)})^T \in \mathbb{R}^{bk \times t}$ are the design matrices of the left and right neighbour effects. For the bk-dimensional random vector e we assume that

$$\mathrm{E}(e) = 0 \quad \text{and} \quad \mathrm{Cov}(e) = \sigma^2 I_{bk}.$$

Additionally, $\beta \in \mathbb{R}^b$, $\tau \in \mathbb{R}^t$, $\lambda \in \mathbb{R}^t$ and $\rho \in \mathbb{R}^t$ denote the vectors of block, direct, left and right neighbour effects, respectively.

For an $n \times m$ matrix A define $\omega^{\perp}(A) = I_n - A(A^TA)^- A^T$ where $(A^TA)^-$ denotes a generalized inverse of A^TA. Then the information matrix for the least squares estimate of τ in model (2.2) is given by

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

see e.g. Kunert (1983).

Assume a design $d^* \in \Omega_{t,b,k}$ is such that C_{d^*} is completely symmetric (that means all its diagonal elements are equal and all its off-diagonal elements are equal) and has maximum trace over all designs $d \in \Omega_{t,b,k}$. Then the design d^* is universally optimal, see Kiefer (1975).

3 An upper bound for $\operatorname{tr} C_d$

Kunert and Martin (2000) determined an upper bound for $\operatorname{tr} C_d$ in the case of 3 and 4 plots per block. Further, they found optimal designs for the case of 3 plots per block and determined highly efficient designs for blocks of size 4. They conjectured that for $t \geq k \geq 5$, a type I orthogonal array will be highly efficient. Extending the work of Kunert and Martin (2000), we are now able to state the following main result.

Theorem 3.1. *For $t \geq k \geq 4$ and any b,*

$$a^*_{t,b,k} = b\left(k - 1 - \frac{(k-1)\left(2k - 3 - \sqrt{4k^2 - 12k + 1}\right)}{k} + \frac{(5 - 3k - 3kt + 3t + k^2t)\left(3 - 2k + \sqrt{4k^2 - 12k + 1}\right)^2}{8kt}\right)$$

is an overall upper bound for $\operatorname{tr} C_d$. The bound is sharp in the sense that, with sufficiently large numbers of blocks, designs are possible that can get arbitrarily close to this bound.

For $k = 4$ the proof of this theorem is implicit in Kunert and Martin (2000). We now prove the case $k \geq 5$.

We begin with some notation. The set of all sequences for t treatments and blocks of size k is

$$\mathfrak{S}(k,t) = \{s = (s_1, \ldots, s_k) : s_j \in \{1, \ldots t\} \quad \forall j = 1, \ldots, k\}\,.$$

We call two sequences s and $\tilde{s}$ equivalent, if we can transform s into $\tilde{s}$ by relabelling the treatments. Thus, $\mathfrak{S}(k,t)$ can be divided into K classes of equivalent sequences. The partial design matrices T_s, L_s and R_s of all sequences from one equivalence class are equal up to permutations of the columns. Thus, for every class $U \subset \mathfrak{S}(k,t)$, we can define

$$\begin{aligned} c_{11}(U) &= \operatorname{tr}\left(T_s^T B_k T_s\right), & c_{12}(U) &= \operatorname{tr}\left(T_s^T B_k L_s\right), \\ c_{13}(U) &= \operatorname{tr}\left(T_s^T B_k R_s\right), & c_{22}(U) &= \operatorname{tr}\left(B_t L_s^T B_k L_s B_t\right), \\ c_{23}(U) &= \operatorname{tr}\left(B_t L_s^T B_k R_s B_t\right), & c_{33}(U) &= \operatorname{tr}\left(B_t R_s^T B_k R_s B_t\right), \end{aligned}$$

where s is an arbitrary sequence in U and $B_k = I_k - {}^1\!/_k 1_k 1_k^T$. For each equivalence class $U \subset \mathfrak{S}(k,t)$, we define the function $H_U \colon \mathbb{R}^2 \to \mathbb{R}$ by

$$H_U(x,y) = c_{11}(U) + 2c_{12}(U)x + 2c_{13}(U)y + c_{22}(U)x^2 + 2c_{23}(U)xy + c_{33}(U)y^2.$$

Then the overall upper bound $a^*_{t,b,k}$ of $\operatorname{tr}(C_d)$ of all designs $d \in \Omega_{t,b,k}$ can be derived from the H_U. More precisely, we determine the function $\max_U H_U(x,y)$ (which is convex) and the number $\min_{(x,y)} \max_U H_U(x,y)$. Then

$$a^*_{t,b,k} = b \min_{(x,y)} \max_U H_U(x,y).$$

This minimum must be attained at a point (x^*, y^*) where either one function H_U has its minimum or where some functions H_{U_r} intersect. Thus, a design d attaining this maximal upper bound $a^*_{t,b,k}$ must consist of sequences from equivalence classes U^* with $H_{U^*}(x^*, y^*) = \max_U H_U(x^*, y^*)$ only. Kunert and Martin (2000) managed to derive those equivalence classes in the case of blocks of size 3 and 4.

For a sequence $s = (s_1, \ldots, s_k) \in \mathfrak{S}(k,t)$ the symmetric complement $s' = (s'_1, \ldots, s'_k) \in \mathfrak{S}(k,t)$ is defined by

$$s'_j = s_{k-j+1} \quad 1 \leq j \leq k.$$

The pair (s, s') is called a symmetric pair of sequences. If $s' = s$, then s is called symmetric. The symmetric complements of all sequences from one equivalence class U all lie in the same equivalence class U'. The class U' is called the symmetric complement of U. The pair (U, U') is called symmetric pair of equivalence classes. If $U = U'$, the class U is called symmetric.

Proposition 3.1. *Consider a symmetric pair of equivalence classes U and U' with representative sequences s and s', respectively. Then*

$$\begin{aligned} c_{11}(U) &= c_{11}(U') & c_{23}(U) &= c_{23}(U') \\ c_{12}(U) &= c_{13}(U') & c_{13}(U) &= c_{12}(U') \\ c_{22}(U) &= c_{33}(U') & c_{33}(U) &= c_{22}(U'). \end{aligned}$$

The proof of this proposition is straightforward, using the fact that $T_{s'}$ is obtained from T_s by simply reordering the rows and columns of T_s.

The symmetry property of the $c_{ij}(U)$ and $c_{ij}(U')$ transfers to the class-specific functions H_U and $H_{U'}$. More precisely

$$H_U(x,y) = H_{U'}(y,x) \quad \forall (x,y).$$

Being the maximum of a finite number of convex functions, $\max_U H_U(x,y)$ is convex and it holds that

$$\max_U H_U(x,y) = \max_{\tilde{U}} H_{\tilde{U}}(y,x) = \max_U H_U(y,x),$$

since the set of all equivalence classes U and the set of all symmetric complements $\tilde{U}$ are equal. That means $\max_U H_U(x,y)$ is symmetric and thus attains its minimum at a point (x^*, y^*), where $x^* = y^*$. Due to this result, we can concentrate our search for $\min_{(x,y)} \max_U H_U(x,y)$ on points (x,y) with $x = y$. Therefore in what follows, we only need to investigate the sequence-specific functions at points $x = y$. Hence, we reduce the functions H_U to functions $\tilde{H}_U : \mathbb{R} \to \mathbb{R}$, defined by

$$\tilde{H}_U(x) = H_U(x,x) \quad \forall x.$$

Note that

$$\tilde{H}_U(x) = c_{11}(U) + 2\left(c_{12}(U) + c_{13}(U)\right) x + \left(c_{22}(U) + 2c_{23}(U) + c_{33}(U)\right) x^2.$$

Using these reduced functions instead of the original ones largely simplifies the computations that follow. Let $s \in \mathfrak{S}(k,t)$ be any sequence of size k for t treatments. For a treatment j we denote by

$n_j(s)$ the number of appearances of treatment j in s,

$\ell_j(s)$ the number of appearances of treatment j in the first $k-1$ plots of s,

$q_j(s)$ the number of appearances of treatment j in the last $k-1$ plots of s,

$m_{jj}(s)$ the number of appearances of treatment j directly followed by itself and

$\tilde{m}_{jj}(s)$ the number of appearances of treatment j followed by itself with one plot in between.

With this notation we get the following formulae for the $c_{ij}(U)$, which will be given without proof.

Proposition 3.2. *Let $U \subset \mathfrak{S}(k,t)$, $t \geq k \geq 5$ be any equivalence class of sequences with representative sequence $s \in U$. With the above notation, it holds that*

$$\begin{aligned}
c_{11}(U) &= k - \frac{1}{k}\sum_{j=1}^{t} n_j(s)^2, \\
c_{12}(U) &= \sum_{j=1}^{t} m_{jj}(s) - \frac{1}{k}\sum_{j=1}^{t} n_j(s)\ell_j(s), \\
c_{13}(U) &= \sum_{j=1}^{t} m_{jj}(s) - \frac{1}{k}\sum_{j=1}^{t} n_j(s)q_j(s), \\
c_{23}(U) &= \sum_{j=1}^{t} \tilde{m}_{jj}(s) - \frac{1}{k}\sum_{j=1}^{t} \ell_j(s)q_j(s) - \frac{1}{t}(k-2) + \frac{1}{tk}(k-1)^2, \\
c_{22}(U) &= (k-1) - \frac{1}{k}\sum_{j=1}^{t} \ell_j(s)^2 - \frac{1}{t}(k-1) + \frac{1}{tk}(k-1)^2, \\
c_{33}(U) &= (k-1) - \frac{1}{k}\sum_{j=1}^{t} q_j(s)^2 - \frac{1}{t}(k-1) + \frac{1}{tk}(k-1)^2.
\end{aligned}$$

Based on these formulae, the reduced sequence-specific function $\tilde{H}_U$ for an equivalence class with representative sequence s becomes

$$\begin{aligned}
\tilde{H}_U(x) = k &- \frac{1}{k}\sum_{j=1}^{t} n_j(s)^2 \\
&+ 2\left(2\sum_{j=1}^{t} m_{jj}(s) - \frac{1}{k}\left(\sum_{j=1}^{k} n_j(s)\ell_j(s) + \sum_{j=1}^{k} n_j(s)q_j(s)\right)\right)x \\
+ &\left(2\sum_{j=1}^{t} \tilde{m}_{jj}(s) - \frac{1}{k}\left(\sum_{j=1}^{t}\left(\ell_j(s)^2 + q_j(s)^2\right)\right) - \frac{2}{k}\sum_{j=1}^{t} \ell_j(s)q_j(s)\right)x^2 \\
+ &\left((k-1)\left(2 - \frac{2}{t}\right) + \frac{2}{tk}(k-1)^2 - \frac{2}{t}(k-1) + \frac{2}{tk}(k-2)^2\right)x^2.
\end{aligned}$$

Kunert and Martin (2000) conjectured that for arbitrary $k \geq 5$ and $t \geq k$, $\min_{x\in\mathbb{R}} \max_{U\in\mathfrak{S}(k,t)} H_U(x)$ is at the intersection of the sequence-specific functions of U_1, U_2, U_3 and U_4, represented by the sequences $s_1 = (1,2,\ldots,k)$, $s_2 = (1,1,2,\ldots,k-1)$, $s_3 = (1,2,\ldots,k-1,k-1)$ and $s_4 = (1,1,2,\ldots,k-3,k-2,k-2)$, respectively. Note that U_3 is the symmetric complement of U_2.

Calculating the corresponding $c_{ij}(U)$, we get the class-specific functions for U_1, U_2, U_3 and U_4 as follows:

$$\begin{aligned}
\tilde{H}_{U_1}(x) &= k - 1 + \left(\frac{4}{k} - 4\right) x + \left(\frac{10 - 6k + 6t - 6kt + 2k^2 t}{kt}\right) x^2 \\
\tilde{H}_{U_2}(x) = \tilde{H}_{U_3}(x) &= k - \frac{2}{k} - 1 - \frac{2}{k} x + \left(\frac{10 - 6k + 2t - 6kt + 2k^2 t}{kt}\right) x^2 \\
\tilde{H}_{U_4}(x) &= k - \frac{4}{k} - 1 + \left(4 - \frac{8}{k}\right) x + \left(\frac{10 - 6k - 2t - 6kt + 2k^2 t}{kt}\right) x^2.
\end{aligned}$$

Defining the function g_k through

$$g_k(x) = 1 - (2k - 3)x + 2x^2,$$

we observe that

$$\tilde{H}_{U_2}(x) = \tilde{H}_{U_1}(x) - \frac{2}{k} g_k(x)$$

and

$$\tilde{H}_{U_4}(x) = \tilde{H}_{U_1}(x) - \frac{4}{k} g_k(x).$$

It follows that all four functions intersect at the roots of the function g_k, namely at the two points

$$\begin{aligned}
x_{1,k} &= \frac{1}{4}\left(2k - 3 - \sqrt{4k^2 - 12k + 1}\right) \quad \text{and} \\
x_{2,k} &= \frac{1}{4}\left(2k - 3 + \sqrt{4k^2 - 12k + 1}\right).
\end{aligned} \tag{3.1}$$

Note that g_k and, therefore, $x_{1,k}$ and $x_{2,k}$ do not depend on the number t of treatments. Since $\tilde{H}_{U_1}(x_{1,k}) < \tilde{H}_{U_1}(x_{2,k})$, we concentrate our investigations on $x_{1,k}$. We want to prove that the common value of $\tilde{H}_{U_i}(x_{1,k})$, $1 \le i \le 4$, really is the minimum of the maxima of all $\tilde{H}_U$. Hence, we have to show that

$$\forall U \subset \mathfrak{S}(k,t): \quad \tilde{H}_U(x_{1,k}) \le \tilde{H}_{U_1}(x_{1,k}) = a_{1,k}, \tag{3.2}$$

say, and that the derivatives of the four class-specific functions $\tilde{H}_{U_i}$, $1 \le i \le 4$, do not all have equal signs in $x_{1,k}$. Note that

$$\begin{aligned}
a_{1,k} = k - 1 &- \frac{(k-1)\left(2k - 3 - \sqrt{4k^2 - 12k + 1}\right)}{k} \\
&+ \frac{(5 - 3k - 3kt + 3t + k^2 t)\left(3 - 2k + \sqrt{4k^2 - 12k + 1}\right)^2}{8kt}
\end{aligned}$$

and

$$x_{1,k} = \frac{1}{4}\left(2k - 3 - 2\sqrt{\left(k - \frac{3}{2}\right)^2 - 2}\right) > \frac{1}{4}\left(2k - 3 - 2\left(k - \frac{3}{2}\right)\right) = 0.$$

Some easy calculations also show that $x_{1,k} \leq x_{1,5} \leq 0.15$.

We start with a consideration of the derivatives.

Proposition 3.3. *For all $k \geq 5$ and all $t \geq k$, we observe that*

$$\begin{aligned}
\tilde{H}'_{U_1}(x_{1,k}) &= 4x_{1,k}\frac{k^2t - kt + 3t - 3k + 5}{kt} - 4\frac{k-1}{k} && < 0,\\
\tilde{H}'_{U_2}(x_{1,k}) &= \tilde{H}'_{U_3}(x_{1,k}) = \tilde{H}'_{U_1}(x_{1,k}) + \frac{2}{k}(2k - 3 - 4x_{1,k}) && > 0,\\
\tilde{H}'_{U_4}(x_{1,k}) &= \tilde{H}'_{U_1}(x_{1,k}) + \frac{4}{k}(2k - 3 - 4x_{1,k}) && > 0.
\end{aligned}$$

Proof. The derivative of $\tilde{H}_{U_1}$ is

$$\tilde{H}'_{U_1}(x) = -4\left(\frac{k-1}{k} - \frac{k^2t - 3kt + 3t - 3k + 5}{kt}x\right).$$

Therefore, $\tilde{H}'_{U_1}(x) = 0$ if and only if

$$x = \frac{k-1}{k^2 - 3k + 3 - \frac{3k-5}{t}} = x_0, \text{ say.}$$

It follows for each t that

$$x_0 \geq \frac{k-1}{k^2 - 3k + 3} = x_0^*, \text{ say.}$$

We then observe that

$$\begin{aligned}
g_k(x_0^*) &= 1 - \frac{(k-1)(2k-3)}{k^2 - 3k + 3} + 2\frac{(k-1)^2}{(k^2 - 3k + 3)^2}\\
&= -\frac{1 + (k-3)(1 + k(k-1)^2)}{(k^2 - 3k + 3)^2} < 0.
\end{aligned}$$

This, however, implies that x_0^* must be inside the interval $(x_{1,k}, x_{2,k})$ and, therefore, $x_0 \geq x_0^* \geq x_{1,k}$. The fact that $\tilde{H}_{U_1}$ is convex, then implies that

$$\tilde{H}'_{U_1}(x_{1,k}) < \tilde{H}'_{U_1}(x_0) = 0.$$

Remembering that

$$\tilde{H}_{U_2}(x) = \tilde{H}_{U_3}(x) = \tilde{H}_{U_1}(x) - \frac{2}{k}g_k(x)$$

and noting that $g'_k(x) = -2k + 3 + 4x$, we get

$$\tilde{H}'_{U_2}(x_{1,k}) = \tilde{H}'_{U_3}(x_{1,k}) = \tilde{H}'_{U_1}(x_{1,k}) + \frac{2}{k}(2k - 3 - 4x_{1,k}).$$

To see that $\tilde{H}'_{U_2}(x_{1,k})$ is positive, we consider the root of $\tilde{H}'_{U_2}$. We get

$$\tilde{H}'_{U_2}(x) = -\frac{2}{k} + 4\frac{k^2t - 3kt + t - 3k + 5}{kt}x,$$

and this is 0 if and only if

$$x = \frac{1}{2(k^2 - 3k + 1 - \frac{3k-5}{t})} = \tilde{x}_0, \text{ say.}$$

Note that for all $t \geq k$ we have

$$\begin{aligned}\tilde{x}_0 &\leq \frac{1}{2(k^2 - 3k + 1 - \frac{3k-5}{k})} \\ &= \frac{1}{2(k^2 - 3k - 2 + \frac{5}{k})} = \tilde{x}_0^*, \text{ say.}\end{aligned}$$

We then calculate that

$$\begin{aligned}g_k(\tilde{x}_0^*) &= \frac{4 + (k-1)\left(24 + (k-2)\left(3 + (k-4)\left(19 + (k-3)(2k^2 + 6k + 9)\right)\right)\right)}{2(k^3 - 3k^2 - 2k + 5)^2} \\ &> 0.\end{aligned}$$

This implies that $\tilde{x}_0^*$ is outside the interval $[x_{1,k}, x_{2,k}]$. Note that $\tilde{x}_0^* < 1$. Since $g_k(1) < 0$, it follows that $\tilde{x}_0 \leq \tilde{x}_0^* < x_{1,k}$. The convexity of $\tilde{H}_{U_2}$ implies that

$$\tilde{H}_{U_2}(x_{1,k}) > \tilde{H}_{U_2}(\tilde{x}_0) = 0.$$

Finally,

$$\tilde{H}'_{U_4}(x) = \tilde{H}'_{U_1}(x) - \frac{4}{k}g_k(x) = \tilde{H}'_{U_2}(x) - \frac{2}{k}g_k(x)$$

and, therefore,

$$\begin{aligned}\tilde{H}'_{U_4}(x_{1,k}) &= \tilde{H}'_{U_1}(x_{1,k}) + \frac{4}{k}(2k - 3 - 4x_{1,k}) \\ &= \tilde{H}'_{U_2}(x_{1,k}) + \frac{2}{k}(2k - 3 - 4x_{1,k}) \\ &> \tilde{H}'_{U_2}(x_{1,k}) > 0.\end{aligned}$$

□

We now prove that $\tilde{H}_U(x_{1,k}) \leq \tilde{H}_{U_1}(x_{1,k})$. We begin with a technical Proposition.

Proposition 3.4. *Consider an arbitrary sequence $s = (s_1, ..., s_k) \in \mathfrak{S}(k,t)$, where not all s_i are the same. Assume that there is one treatment 1, say, appearing more than once in s, and that at least one appearance of treatment 1 is in the inside, i.e. on one of the plots $2, \ldots, k-1$. Then there must be another treatment 2, say, which does not appear* *at all in s. Now construct sequence $\tilde{s}$ from s by replacing one appearance of treatment 1 in an inside plot by treatment 2. For this replacement, choose a plot receiving treatment 1, where either the preceding or the ensuing plot receives another treatment than 1. We then find for classes U containing s and $\tilde{U}$ containing $\tilde{s}$ that*

$$\begin{aligned}
&c_{11}(\tilde{U}) - c_{11}(U) = \frac{2}{k}(n_1(s) - 1),\\
&c_{12}(\tilde{U}) - c_{12}(U) + c_{13}(\tilde{U}) - c_{13}(U)\\
&\qquad = 2\left(m_{11}(\tilde{s}) - m_{11}(s)\right) + \frac{1}{k}\left(2n_1(s) + \ell_1(s) + q_1(s) - 4\right) \quad \textit{and}\\
&c_{22}(\tilde{U}) - c_{22}(U) + 2c_{23}(\tilde{U}) - 2c_{23}(U) + c_{33}(\tilde{U}) - c_{33}(U)\\
&\qquad = 2\left(\tilde{m}_{11}(\tilde{s}) - \tilde{m}_{11}(s)\right) + \frac{1}{k}\left(4\left(\ell_1(s) + q_1(s)\right) - 8\right).
\end{aligned}$$

Proof. Observe that the transformation of s to $\tilde{s}$ implies that for all $3 \le i \le t$ we have

$$\begin{aligned}
n_i(\tilde{s}) &= n_i(s), & \ell_i(\tilde{s}) &= \ell_i(s), & q_i(\tilde{s}) &= q_i(s),\\
m_{ii}(\tilde{s}) &= m_{ii}(s), \quad \text{and} & \tilde{m}_{ii}(\tilde{s}) &= \tilde{m}_{ii}(s).
\end{aligned}$$

For $i = 1$ and $i = 2$, however, there are differences. We get that

$$\begin{aligned}
n_1(\tilde{s}) &= n_1(s) - 1, & \ell_1(\tilde{s}) &= \ell_1(s) - 1,\\
q_1(\tilde{s}) &= q_1(s) - 1, & m_{11}(\tilde{s}) &\in \{m_{11}(s), m_{11}(s) - 1\},\\
m_{22}(\tilde{s}) &= \tilde{m}_{22}(\tilde{s}) = 0, & \tilde{m}_{11}(\tilde{s}) &\in \{\tilde{m}_{11}(s), \tilde{m}_{11}(s) - 1, \tilde{m}_{11}(s) - 2\},
\end{aligned}$$

and

$$\begin{aligned}
&n_2(s) = \ell_2(s) = q_2(s) = m_{22}(s) = \tilde{m}_{22}(s) = 0 \quad \text{and}\\
&n_2(\tilde{s}) = \ell_2(\tilde{s}) = q_2(\tilde{s}) = 1.
\end{aligned}$$

The proposition then follows by direct calculation. □

Note that in Proposition 3.4 we have excluded sequences like (1,1,...,1).

Proposition 3.5. *If the sequence s from Proposition 3.4 is in class U and the sequence $\tilde{s}$ is in class $\tilde{U}$, then*

$$\tilde{H}_{\tilde{U}}(x_{1,k}) \ge \tilde{H}_U(x_{1,k}).$$

Proof. Making use of Proposition 3.4, it is easy to see that

$$\begin{aligned}
\tilde{H}_{\tilde{U}}(x) - \tilde{H}_U(x) &= c_{11}(\tilde{U}) - c_{11}(U) \\
&\quad + 2x\left(c_{12}(\tilde{U}) - c_{12}(U) + c_{13}(\tilde{U}) - c_{13}(U)\right) \\
&\quad + x^2\left(c_{22}(\tilde{U}) - c_{22}(U) + c_{33}(\tilde{U}) - c_{33}(U)\right) \\
&\quad + 2x^2\left(c_{23}(\tilde{U}) - c_{23}(U)\right) \\
&= \frac{2}{k}(n_1(s) - 1) \\
&\quad + 2x\left(2m_{11}(\tilde{s}) - 2m_{11}(s) + \frac{1}{k}(2n_1(s) + \ell_1(s) + q_1(s) - 4\right) \\
&\quad + x^2\left(2\tilde{m}_{11}(\tilde{s}) - 2\tilde{m}_{11}(s) + \frac{1}{k}(4\ell_1(s) + 4q_1(s) - 8)\right)
\end{aligned}$$

To continue, we distinguish between several cases.

Case 1: $\tilde{m}_{11}(\tilde{s}) = \tilde{m}_{11}(s)$.

Remember that $x_{1,k} > 0$, $n_1(s) \geq 2$ and $m_{11}(\tilde{s}) \geq m_{11}(s) - 1$. Further, note that $\ell_1(s) + q_1(s) \geq 3$. Therefore, it follows that

$$\begin{aligned}
\tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &\geq \frac{2}{k} + 2x_{1,k}(-2 + \frac{1}{k}(4 + 3 - 4)) \\
&\quad + x_{1,k}^2(\frac{1}{k}(4 \times 3 - 8)) \\
&= \frac{2}{k}\left(1 - (2k - 3)x_{1,k} + 2x_{1,k}^2\right) \\
&= 0,
\end{aligned}$$

by the definition of $x_{1,k}$.

Case 2: $m_{11}(\tilde{s}) = m_{11}(s)$.

Remember that $\tilde{m}_{11}(\tilde{s}) \geq \tilde{m}_{11}(s) - 2$. Then, similarly to case 1, it follows that

$$\begin{aligned}
\tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &\geq \frac{2}{k} + 2x_{1,k}(\frac{1}{k}(4 + 3 - 4)) \\
&\quad + x_{1,k}^2(-4 + \frac{1}{k}(4 \times 3 - 8))
\end{aligned}$$

Since $x_{1,k} \geq x_{1,k}^2$, it follows that

$$\begin{aligned}
\tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &\geq \frac{2}{k} + 2x_{1,k}(-2 + \frac{1}{k}(4 + 3 - 4)) \\
&\quad + x_{1,k}^2(\frac{1}{k}(4 \times 3 - 8)) \\
&= \frac{2}{k}\left(1 - (2k - 3)x_{1,k} + 2x_{1,k}^2\right) \\
&= 0,
\end{aligned}$$

as in case 2.

Case 3: $m_{11}(\tilde{s}) = m_{11}(s) - 1$ and $\tilde{m}_{11}(\tilde{s}) \leq \tilde{m}_{11}(s) - 1$.
This is only possible if we have at least three consecutive appearances of treatment 1. Therefore, we have $n_1(s) \geq 3$, $\ell_1(s) + q_1(s) \geq 5$. It then follows that

$$\begin{aligned}\tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &\geq \frac{2}{k}(3-1) \\ &\quad + 2x_{1,k}\left(-2 + \frac{1}{k}(6+5-4)\right) \\ &\quad + x_{1,k}^2\left(-4 + \frac{1}{k}(20-8)\right) \\ &= \frac{2}{k}\left(2 + x_{1,k}(7-2k) + x_{1,k}^2(6-2k)\right).\end{aligned}$$

Remember that $x_{1,k}$ is a root of the function g, where

$$g(x) = 1 - (2k-3)x + 2x^2.$$

Therefore,

$$\begin{aligned}\tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &= \tilde{H}_{\tilde{U}}(x_{1,k}) - \tilde{H}_U(x_{1,k}) - \frac{4}{k}g(x_{1,k}) \\ &= \frac{2}{k}\big(2 + x_{1,k}(7-2k) + x_{1,k}^2(6-2k) \\ &\quad -2 - x_{1,k}(6-4k) - x_{1,k}^2 \times 4\big) \\ &= \frac{2}{k}\left(x_{1,k}(1+2k) + x_{1,k}^2(2-2k)\right) \\ &\geq \frac{2}{k}x_{1,k} \times 3 \geq 0,\end{aligned}$$

where we have used again that $x_{1,k} \geq x_{1,k}^2$.

This completes the proof. $\square$

These technical propositions can now be used to prove the main result.

Proposition 3.6. *Consider an arbitrary sequence s with k plots and t treatments and denote by U the equivalence class to which s belongs. Further consider equivalence class U_1 containing the sequence $s_1 = (1, 2, 3, \ldots, k)$. Then*

$$\tilde{H}_{U_1}(x_{1,k}) \geq \tilde{H}_U(x_{1,k}).$$

Proof. If s is such that each treatment appears at most once, then s is in class U_1. Now assume that s is such that treatment 1, say, appears more than once. Then we consider three cases.

Case 1: $s = (1, 1, 1, \dots, 1)$.
In that case,

$$\tilde{H}_U(x) = \frac{2kt - 2t + 2k + 2}{kt}\, x^2.$$

Therefore,

$$\begin{aligned}
\tilde{H}_{U_1}(x_{1,k}) - \tilde{H}_U(x_{1,k}) &= k - 1 + \left(\frac{4}{k} - 4\right) x_{1,k} \\
&\quad + \frac{8kt + 4t - 4k - 8 + 2k^2 t}{kt} x_{1,k}^2 \\
&\geq k - 1 + \left(\frac{4}{k} - 4\right) x_{1,k} + 2kx_{1,k}^2 \\
&\geq k - 1 - 4 + 2kx_{1,k}^2 \geq 0,
\end{aligned}$$

so

$$\tilde{H}_U(x_{1,k}) \leq \tilde{H}_{U_1}(x_{1,k}).$$

Case 2: s fulfills the conditions of Proposition 3.4.
According to Proposition 3.4, we derive sequence $\tilde{s}$, where $\tilde{s}$ contains once repetition of treatment 1 less than s. According to Proposition 3.5 we observe for the equivalence class $\tilde{U}$ containing $\tilde{s}$ that $\tilde{H}_{\tilde{U}}(x_{1,k}) \geq \tilde{H}_U(x_{1,k})$.

We then can apply Propositions 3.4 and 3.5 on $\tilde{s}$ iteratively, until we either end up in sequence $s_1 = (1, 2, 3, \dots, k)$, or in sequence $s^* = (1, 2, \dots, k-1, 1)$.

Case 3: s is equivalent to $s^* = (1, 2, \dots, k-1, 1)$.
In that case,

$$\begin{aligned}
n_i(s_1) = n_i(s^*) &= 1, \quad \text{for all} \quad 2 \leq i \leq k-1, \\
\ell_i(s_1) = \ell_i(s^*) &= 1, \quad \text{for all} \quad 2 \leq i \leq k-1, \\
q_i(s_1) = q_i(s^*) &= 1, \quad \text{for all} \quad 2 \leq i \leq k-1, \\
m_{ii}(s_1) = m_{ii}(s^*) &= 0, \quad \text{for all} \quad 1 \leq i \leq k, \\
\tilde{m}_{ii}(s_1) = \tilde{m}_{ii}(s^*) &= 0, \quad \text{for all} \quad 1 \leq i \leq k,
\end{aligned}$$

while

$$\begin{array}{llll}
n_1(s_1) = 1, & n_1(s^*) = 2, & n_k(s_1) = 1, & n_k(s^*) = 0, \\
q_1(s_1) = 0, & q_1(s^*) = 1, & q_k(s_1) = 1, & q_k(s^*) = 0,
\end{array}$$

and

$$\ell_k(s_1) = \ell_k(s^*) = 0 \quad \text{and} \quad \ell_1(s_1) = \ell_1(s^*) = 1.$$

This implies that

$$
\begin{aligned}
&c_{11}(s_1) - c_{11}(s^*) = \frac{2}{k}, \\
&c_{12}(s_1) - c_{12}(s^*) + c_{13}(s_1) - c_{13}(s^*) = \frac{2}{k}, \\
&c_{22}(s_1) - c_{22}(s^*) + 2c_{23}(s_1) - 2c_{23}(s^*) + c_{33}(s_1) - c_{33}(s^*) = \frac{4}{k},
\end{aligned}
$$

and, therefore, $\tilde{H}_{U_1}(x_{1,k}) \geq \tilde{H}_U(x_{1,k})$.

This completes the proof. □

Using Propositions 3.2 to 3.6, Theorem 3.1 is proven for any $t \geq k \geq 5$ and given number b of blocks, with $b * a_{1,k} = a^*_{t,b,k}$.

To achieve that $\operatorname{tr} C_d = a^*_{t,b,k}$ for a design d, it can use sequences from the classes U_1, U_2, U_3 and U_4 only. The proportions $\pi_{d,i}, 1 \leq i \leq 4$, of sequences U_1, U_2, U_3 and U_4 must be such that

$$\sum_{i=1}^{4} \pi_{d,i} \tilde{H}'_{U_i}(x_{1,k}) = 0.$$

We know from Proposition 3.3 that $\tilde{H}'_{U_1}(x_{1,k})$ is negative, while the other three $\tilde{H}'_{U_i}(x_{1,k})$ are positive. Therefore, we have two basic possibilities. Either

$$\pi_{d,1} = \frac{H'_{U_4}(x_{1,k})}{H'_{U_4}(x_{1,k}) - H'_{U_1}(x_{1,k})},$$

with $\pi_{d,4} = 1 - \pi_{d,1}$ and $\pi_{d,2} = \pi_{d,3} = 0$, or

$$\pi_{d,1} = \frac{H'_{U_2}(x_{1,k})}{H'_{U_2}(x_{1,k}) - H'_{U_1}(x_{1,k})},$$

with $\pi_{d,2} = \pi_{d,3} = \frac{1-\pi_{d,1}}{2}$ and $\pi_{d,4} = 0$. Any convex combination of these two possibilities would also be possible. Furthermore, we need to chose the sequences in such a way that all C_{dij} are completely symmetric.

Like in Kunert and Martin (2000), the desired proportions are generally not rational numbers. Therefore, we are not able to construct these designs for finite numbers of blocks. Nevertheless, note that if the number b of blocks tends to infinity, the proposed bound is achieved. We can construct efficient designs, like Kunert and Martin (2000), or we can make use of orthogonal arrays of type I, which achieve high efficiencies under any Φ_p-criterion.

4 Efficiency of orthogonal arrays of type I

An $OA_I(b, k, t, 2)$ uses sequences from equivalence class U_1 only and has a completely symmetric C_d. The Φ_p-criterion of any a design d is

$$\Phi_p(C_d) = \left(\frac{\sum_{i=1}^{t-1} \mu_{di}^{-p}}{t-1} \right)^{1/p},$$

where μ_{di}, $i = 1, \dots t-1$ denotes the $t-1$ nonzero eigenvalues of C_d. If d is an $OA_I(b, k, t, 2)$, then C_d is completely symmetric, see Martin and Eccelston (2004). Therefore, $\mu_{d1} = \dots = \mu_{dt-1} = \operatorname{tr} C_d (t-1)^{-1}$ and we get that

$$\Phi_p(C_d) = \frac{t-1}{\operatorname{tr} C_d},$$

see Kunert (1987). Thus, a lower bound for the efficiency of an orthogonal array of type I for t treatments and k plots per block is given by

$$\text{Eff}(k, t) = \frac{\operatorname{tr} C_d}{a^*_{t,b,k}}.$$

It is easy to see that for any given $k \geq 5$, $\text{Eff}(k, t)$ is monotonously increasing in $t \geq k$. Further, $\text{Eff}(k, k)$ is monotonously increasing in k. Thus for all $t \geq k \geq 5$, we get that

$$\text{Eff}(k, t) \geq \text{Eff}(5, 5) \approx 0.94.$$

More specific, we get efficiencies of 0.94, 0.97 and 0.98 for $k = t = 5$, $k = t = 6$ and $k = t = 7$, respectively and accordingly higher values for other combinations of $t \geq k \geq 5$.

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