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Katarzyna Filipiak, Rafal Rózański, Aneta Sawikowska, Dominika Wojtera-Tyrakowska. On the E-optimality of complete designs under an interference model. *Statistics and Probability Letters*, 2009, 78 (15), pp.2470. 10.1016/j.spl.2008.02.038 . hal-00586130

HAL Id: hal-00586130

<https://hal.science/hal-00586130>

Submitted on 15 Apr 2011

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Accepted Manuscript

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PII: S0167-7152(08)00151-X
DOI: [10.1016/j.spl.2008.02.038](https://doi.org/10.1016/j.spl.2008.02.038)
Reference: STAPRO 5001

To appear in: *Statistics and Probability Letters*

Received date: 8 February 2007
Revised date: 16 January 2008
Accepted date: 14 February 2008

Please cite this article as: Filipiak, K., Róžański, R., Sawikowska, A., Wojtera-Tyrakowska, D., On the E-optimality of complete designs under an interference model. *Statistics and Probability Letters* (2008), doi:10.1016/j.spl.2008.02.038

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On the E-optimality of complete designs under an interference model

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Abstract

In the experiments in which the response to a treatment can be affected by other treatments, the interference model with neighbor effects is usually applied. It is known, that circular neighbor balanced designs (CNBD) are universally optimal under this model. However, such designs cannot exist for each combination of design parameters. If in the class of block designs with a given number of blocks there exists CNBD, then such a design cannot exist in the class with one block less or more. The aim of this paper is to identify the E-optimal complete block designs under the interference model with neighbor effects over such classes of designs. The results are based on algebraic properties of information matrix.

Keywords: Interference model, Information matrix, E-optimal designs, Spectral norm, Reducible matrices

¹Research partially supported by the Interdisciplinary Joint Research Project 2004/2005 of Adam Mickiewicz University and Agricultural University of Poznań.

1 Introduction

In the theory of experimental designs, the problem of determining optimal designs is often considered. If in an experiment the response to a treatment is affected by other treatments (for example in agricultural and horticultural experiments), then the optimality of designs under an interference model is studied. Recently some results on universal optimality of binary designs under this model were published. These results concern mainly optimality of circular neighbor balanced designs (CNBD) and orthogonal arrays of type I under the fixed and mixed interference models, where the observations are correlated or not (see e.g. Druilhet, 1999, Filipiak and Markiewicz, 2003, 2004, 2005, 2007). It is known, however, that for some combinations of design parameters the universally optimal designs cannot exist. In such a case efficiency of some designs or optimality with respect to the specified criteria are considered. The efficiency of some cyclic designs under a fixed interference model was studied in Filipiak and Rózański, 2004.

In this paper we are interested in determining E-optimal designs under an interference model. This criterion is based on the eigenvalues of the information matrices of designs. In the literature this problem has not been discussed yet. Only the problem of determining E-optimal designs under the model with block effects as the only nuisance parameters over the class of designs is partially solved, see e.g. Constantine, 1981, Jacroux, 1982, 1983, Srivastav and Shankar, 2003. However, there is no characterization of E-optimal designs under an interference model.

It is known, that in the class of block designs with the same number of treatments, t , as block sizes, k , CNBD cannot exist for the number of blocks $b = t - 2$ and $b = t$. Thus, for such design parameters we determine the structure of left-neighboring matrix of E-optimal design under the interference model with left-neighbor effects and we give some examples of such designs.

It is worth observing that designs with $t = k$ are often used in practice. For example in UPOV (The International Union for the Protection of New Varieties of Plants) research, complete block designs are recommended in experiments when the number of treatments is less than 16. The designs with the same number of blocks as number of treatments and units are also applied in clinical trials.

This paper is organized as follows. First we present some general definitions and notation. In Section 3 we characterize the structure of the left-neighboring matrix of E-optimal design with $t = k = b$. In Section 4 we determine the structure of the left-neighboring matrix of E-optimal design with $t = k = b + 2$. In the last section we give the method of construction of E-optimal designs and some examples.

2 Definitions and notations

Let $\mathcal{D}_{t,b,k}$ be the set of designs with t treatments, b blocks and k experimental units per block. An interference model with left-neighbor effects associated with the design $d \in \mathcal{D}_{t,b,k}$ can be written as

$$\mathbf{y} = \mathbf{T}_d \boldsymbol{\tau} + \mathbf{L}_d \boldsymbol{\lambda} + (\mathbf{I}_b \otimes \mathbf{1}_k) \boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad (1)$$

where $\boldsymbol{\tau}$, $\boldsymbol{\lambda}$ and $\boldsymbol{\beta}$ are the vectors of treatment effects, left-neighbor effects and block effects, respectively. Here $\boldsymbol{\varepsilon}$ is a vector of random errors with $E(\boldsymbol{\varepsilon}) = \mathbf{0}$ and $\text{Cov}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}_{bk}$, where σ^2 is an unknown constant. The matrix \mathbf{I}_b denotes the identity matrix of order b , $\mathbf{1}_k$ is the k -vector of ones and \otimes denotes the Kronecker product.

Let \mathbf{T}_{du} be the design matrix of treatment effects in block u , $1 \leq u \leq b$. Further, define $\mathbf{T}_d = (\mathbf{T}'_{d1} : \cdots : \mathbf{T}'_{db})'$ as the design matrix of treatment effects. For each u we define $\mathbf{L}_{du} = \mathbf{H}_k \mathbf{T}_{du}$, where \mathbf{H}_k is a $k \times k$ matrix of the form

$$\mathbf{H}_k = \begin{pmatrix} \mathbf{0}'_{k-1} & 1 \\ \mathbf{I}_{k-1} & \mathbf{0}_{k-1} \end{pmatrix}. \quad (2)$$

Then, $\mathbf{L}_d = (\mathbf{I}_b \otimes \mathbf{H}_k) \mathbf{T}_d$ is the design matrix of left-neighbor effects. This form of the matrix \mathbf{H}_k follows from the assumption that each treatment has a left neighbor. This situation may occur if each block of a design has the form of a circle. If plots in blocks are arranged in linear forms, we can obtain the effect of circularity by adding *border plots* at the beginning of each block, where the treatment at the border plot is the same as the treatment at the opposite end of the block (for more details see e.g. Druilhet, 1999, Filipiak and Rózański, 2005). Border plots are not used for measuring the response variables.

Under the interference model (1), the information matrix for estimating the treatment effects, \mathbf{C}_d , can be expressed as

$$\mathbf{C}_d = \mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{T}_d - \mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{L}_d (\mathbf{L}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{L}_d)^{-1} \mathbf{L}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{T}_d, \quad (3)$$

where $\mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k}$ is the orthogonal projector onto the orthocomplement of the column span of $\mathbf{I}_b \otimes \mathbf{1}_k$ and \mathbf{A}^- denotes a generalized inverse of \mathbf{A} . It is easy to see that $\mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} = \mathbf{I}_b \otimes \mathbf{E}_k$, where $\mathbf{E}_k = \mathbf{I}_k - \frac{1}{k} \mathbf{1}_k \mathbf{1}'_k$. Because of the form of \mathbf{E}_k and since \mathbf{H}_k is orthogonal, it can be seen that $\mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{T}_d = \mathbf{L}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{L}_d$.

We are interested in determining E-optimal design, i.e. such design, that the maximal variance among all best linear unbiased estimators of normalized linear contrasts is minimal under this design. The condition of E-optimality can be expressed in terms of eigenvalues of the information matrix as follows.

For a design $d \in \mathcal{D}_{t,b,k}$ let $\lambda_{max}(\mathbf{C}_d) = \lambda_1(\mathbf{C}_d) \geq \lambda_2(\mathbf{C}_d) \geq \cdots \geq \lambda_{t-1}(\mathbf{C}_d) \geq \lambda_t(\mathbf{C}_d) = 0$ be the eigenvalues of its information matrix \mathbf{C}_d . A design $d^* \in \mathcal{D}_{t,b,k}$ is called *E-optimal* over $\mathcal{D}_{t,b,k}$ if $\lambda_{t-1}(\mathbf{C}_{d^*}) \geq \lambda_{t-1}(\mathbf{C}_d)$ for all designs $d \in \mathcal{D}_{t,b,k}$ (cf. Constantine, 1981).

Observe, that in formula (3) it is involved a generalized inverse of a matrix, which depends on a design, i.e. which changes itself with the arrangement of treatments on experimental units. It makes the determination of E-optimal design difficult. Therefore in this paper we consider experiments with $t = k$ ($t > 2$). The class of designs with $t = k$, in which each treatment occurs at most once in each block (the class of complete binary designs) we will denote by $\mathcal{B}_{t,b,t}$. In such a case the information matrix has the form

$$\mathbf{C}_d = b\mathbf{E}_t - \frac{1}{b}\mathbf{K}_d\mathbf{K}'_d,$$

where $\mathbf{K}_d = \mathbf{T}'_d\mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_t}\mathbf{L}_d$. Since the vectors $\mathbf{T}_d\mathbf{1}_t$ and $\mathbf{L}_d\mathbf{1}_t$ are in the column space of $\mathbf{I}_b \otimes \mathbf{1}_t$, the matrix \mathbf{K}_d has zero row and column sums, i.e. $\mathbf{K}_d\mathbf{1}_t = \mathbf{K}'_d\mathbf{1}_t = \mathbf{0}_t$, where $\mathbf{0}_t$ is a t -vector of zeros.

Observe that the matrix \mathbf{E}_t is symmetric, idempotent and $t - 1$ of its eigenvalues are equal to 1. Moreover, $\mathbf{E}_t\mathbf{1}_t = \mathbf{0}_t$ and $\mathbf{K}_d\mathbf{K}'_d\mathbf{1}_t = \mathbf{0}_t$. Thus, under the class $\mathcal{B}_{t,b,t}$, the E-optimality condition can be rewritten as follows

$$\lambda_1(\mathbf{K}_{d^*}\mathbf{K}'_{d^*}) \leq \lambda_1(\mathbf{K}_d\mathbf{K}'_d) \quad \text{for all } d \in \mathcal{B}_{t,b,t}. \quad (4)$$

Since for a nonnegative-definite matrix \mathbf{A} , $\sqrt{\lambda_1(\mathbf{A}\mathbf{A}')} = \sigma_1(\mathbf{A})$, where $\sigma_1(\mathbf{A})$ denotes the spectral norm of \mathbf{A} , to determine E-optimal design d^* we have to find the matrix \mathbf{K}_{d^*} with minimal spectral norm over matrices \mathbf{K}_d , $d \in \mathcal{B}_{t,b,t}$. We use some special properties of \mathbf{K}_d .

Using the form of $\mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_t}$, the matrix \mathbf{K}_d can be expressed as $\mathbf{T}'_d\mathbf{L}_d - \frac{b}{t}\mathbf{1}_t\mathbf{1}'_t$. The (i, j) th entry of $\mathbf{T}'_d\mathbf{L}_d$ denotes the number of occurrences of treatment i with treatment j as left neighbor in a design $d \in \mathcal{B}_{t,b,t}$. Therefore we will call this matrix a *left-neighboring matrix* and we will denote it by \mathbf{S}_d with entries s_{ij} , $i, j = 1, 2, \dots, t$. It is easy to observe, that in the class $\mathcal{B}_{t,b,t}$, the diagonal entries of \mathbf{S}_d are equal to 0 and the off-diagonal entries belong to the set $\{0, 1, \dots, b\}$. Moreover, $\mathbf{S}_d\mathbf{1}_t = \mathbf{S}'_d\mathbf{1}_t = b\mathbf{1}_t$. Thus, the set of all matrices \mathbf{K}_d for $d \in \mathcal{B}_{t,b,t}$ can be defined as

$$\mathcal{K}_b = \left\{ \mathbf{K}_d = (k_{ij})_{1 \leq i, j \leq t} : \mathbf{K}_d\mathbf{1}_t = \mathbf{K}'_d\mathbf{1}_t = \mathbf{0}_t, k_{ij} \in \left\{ -\frac{b}{t}, 1 - \frac{b}{t}, \dots, b - \frac{b}{t} \right\}, k_{ii} = -\frac{b}{t} \right\}.$$

Let \mathcal{P}_t be the set of all permutation matrices of order t and let $\overline{\mathcal{P}}_t \subset \mathcal{P}_t$ be the set of permutation matrices with zero diagonal (the set of derangement matrices). We show that the matrix \mathbf{K}_{d^*} with minimal spectral norm over \mathcal{K}_b belongs to the set

$$\tilde{\mathcal{K}}_t = \{ \mathbf{K}_d \in \mathcal{K}_t : \mathbf{K}_d = \mathbf{P}_d - \mathbf{I}_t, \mathbf{P}_d \in \overline{\mathcal{P}}_t \} \quad \text{if } b = t$$

and

$$\hat{\mathcal{K}}_{t-2} = \left\{ \mathbf{K}_d \in \mathcal{K}_{t-2} : \mathbf{K}_d = \frac{2}{t}\mathbf{1}_t\mathbf{1}'_t - \mathbf{I}_t - \mathbf{P}_d, \mathbf{P}_d \in \overline{\mathcal{P}}_t \right\} \quad \text{if } b = t - 2.$$

We prove that design d^* which is E-optimal over $\mathcal{B}_{t,b,t}$, i.e. design for which \mathbf{K}_{d^*} has minimal spectral norm over \mathcal{K}_b , is also E-optimal over $\mathcal{D}_{t,b,t}$.

In the paper reducibility of matrices, will play an important role. Reducibility is defined as follows.

Definition 2.1 (*Horn and Johnson, 1985*). An $n \times n$ matrix \mathbf{A} is said to be reducible if either of the following conditions is satisfied

1. $n = 1$ and $\mathbf{A} = 0$,
2. $n \geq 2$ and there is a permutation matrix $\mathbf{P} \in \mathcal{P}_n$ and an integer r with $1 \leq r \leq n - 1$ such that $\mathbf{P}'\mathbf{A}\mathbf{P} = \begin{bmatrix} \mathbf{B} & \mathbf{C} \\ \mathbf{\Theta} & \mathbf{D} \end{bmatrix}$, where $\mathbf{B} \in \mathbb{C}^{r \times r}$, $\mathbf{D} \in \mathbb{C}^{(n-r) \times (n-r)}$, $\mathbf{C} \in \mathbb{C}^{r \times (n-r)}$ and $\mathbf{\Theta} \in \mathbb{C}^{(n-r) \times r}$ is a zero matrix.

A matrix is called irreducible if it is not reducible.

The matrix $\mathbf{P}'\mathbf{A}\mathbf{P}$, where $\mathbf{P} \in \mathcal{P}_n$, is called the matrix *permutationally similar* to \mathbf{A} . Recall, that the eigenvalues of \mathbf{A} and a matrix permutationally similar to \mathbf{A} are the same.

Observe, that every irreducible derangement matrix is permutationally similar to the matrix \mathbf{H}_t , defined in (2). Moreover, all reducible derangement matrices are permutationally similar to the block diagonal matrices with derangement matrices on the diagonal. It is worth to note, that the eigenvalues of each matrix permutationally similar to \mathbf{H}_t are equal to ω_k , $k = 0, 1, \dots, t-1$, where ω_k are t th roots of unity. It follows from circularity of \mathbf{H}_t (for more details see e.g. Horn and Johnson, 1985, John, 1987).

In this paper we consider $b = t - 2$ and $b = t$, because for the remaining numbers of blocks determining the spectral norm of \mathbf{K}_d requires the spectral norm of two (or more) different permutation matrices, which is very difficult to solve in general.

3 E-optimal designs over $\mathcal{D}_{t,t,t}$

In this section we determine the structure of the left-neighboring matrix of E-optimal design over $\mathcal{D}_{t,t,t}$. First we determine, which structure of \mathbf{K}_d from $\tilde{\mathcal{K}}_t$ gives the minimal spectral norm over \mathcal{K}_t . Then we show the structure of the left-neighboring matrix of E-optimal design over the class of binary designs $\mathcal{B}_{t,t,t}$ and, finally, over the class of all designs $\mathcal{D}_{t,t,t}$.

Observe that a matrix $\mathbf{K}_d \in \tilde{\mathcal{K}}_t$ is reducible if and only if it is permutationally similar to the block-diagonal matrix $\text{diag}(\mathbf{H}_{t_1}, \mathbf{H}_{t_2}, \dots, \mathbf{H}_{t_n}) - \mathbf{I}_t$, where $\sum_{j=1}^n t_j = t$ and $n \neq 1$. It is obvious that for $n = 1$ we obtain an irreducible matrix.

Since the sets of eigenvalues of permutationally similar matrices are the same, the problem of finding the matrix from $\tilde{\mathcal{K}}_t$ with minimal spectral norm can be reduced to studying the spectral norms of $\mathbf{H}_t - \mathbf{I}_t$ or $\text{diag}(\mathbf{H}_{t_1}, \mathbf{H}_{t_2}, \dots, \mathbf{H}_{t_n}) - \mathbf{I}_t$.

Consider a matrix $\mathbf{K}_d = \mathbf{H}_t - \mathbf{I}_t$. Then $\mathbf{K}_d \mathbf{K}_d' = 2\mathbf{I}_t - (\mathbf{H}_t + \mathbf{H}_t') = 2\mathbf{I}_t - (\mathbf{H}_t + \mathbf{H}_t^{-1})$ is circular and its eigenvalues are equal to $2 - \omega_k - \omega_k^{-1} = 2 - 2 \cos \frac{2k\pi}{t}$, $k = 0, 1, \dots, t-1$

(cf. John, 1987). It is easy to see that $\lambda_{max}(\mathbf{K}_d\mathbf{K}'_d)$ is obtained for $k = \frac{t}{2}$ for even t and $k = \frac{t\pm 1}{2}$ for odd t and

$$\lambda_{max}(\mathbf{K}_d\mathbf{K}'_d) = \begin{cases} 2 - 2 \cos \pi = 4 & \text{for even } t \\ 2 - 2 \cos \frac{(t\pm 1)\pi}{t} = 2 + 2 \cos \frac{\pi}{t} & \text{for odd } t. \end{cases} \quad (5)$$

Moreover, it is easy to see that for odd t

$$\lim_{t \rightarrow \infty} \cos \frac{\pi}{t} = 1, \quad (6)$$

and $\lambda_{max}(\mathbf{K}_d\mathbf{K}'_d) \rightarrow 4^-$ if $t \rightarrow \infty$.

Since $\sigma_1(\mathbf{K}_d) = \sqrt{\lambda_{max}(\mathbf{K}_d\mathbf{K}'_d)}$, for $\mathbf{K}_d = \mathbf{H}_t - \mathbf{I}_t$ we get $\sigma_1(\mathbf{K}_d) = 2$ for even t and $\sigma_1(\mathbf{K}_d) \rightarrow 2^-$ if t is odd and $t \rightarrow \infty$.

Recall, that the spectrum of the block-diagonal matrix is the sum of the spectra of diagonal blocks (see e.g. Marcus and Minc, 1964). From the block-diagonal form of the reducible matrices from $\tilde{\mathcal{K}}_t$ it is easy to see that the matrix $\mathbf{K}_d\mathbf{K}'_d$ is also block-diagonal and we can prove the following theorem.

Theorem 3.1 *The matrix \mathbf{K}_{d^*} which minimizes the spectral norm over \mathcal{K}_t is permutationally similar to the matrix:*

- (i) $\mathbf{H}_t - \mathbf{I}_t$ if $t = 2, 7$;
- (ii) $\mathbf{I}_2 \otimes \mathbf{H}_2 - \mathbf{I}_4$ or $\mathbf{H}_4 - \mathbf{I}_4$ if $t = 4$;
- (iii) $\mathbf{I}_m \otimes \mathbf{H}_3 - \mathbf{I}_t$ if $t = 3m, m \in \mathbb{N}$;
- (iv) $\text{diag}(\mathbf{I}_i \otimes \mathbf{H}_3, \mathbf{I}_j \otimes \mathbf{H}_5) - \mathbf{I}_t$ if $t = 5$ or $t \geq 8$ and $t \neq 3m, m \in \mathbb{N}$, where $t = 3i + 5j$ for some $i \in \mathbb{N} \cup \{0\}, j \in \mathbb{N}$.

Moreover, in case (iii) there is $\sigma_1(\mathbf{K}_{d^*}) = \sqrt{3}$ and the spectrum of $\mathbf{K}_{d^*}\mathbf{K}'_{d^*}$ has the form $\underbrace{\{0, 0, \dots, 0\}}_{m \text{ times}}, \underbrace{\{3, 3, \dots, 3\}}_{2m \text{ times}}$, and in case (iv) the spectral norm of \mathbf{K}_{d^*} is $\sigma_1(\mathbf{K}_{d^*}) = \sqrt{\frac{5+\sqrt{5}}{2}}$.

Proof.

Let $\mathbf{K}_d \in \tilde{\mathcal{K}}_t$. From (5) it is easy to see that the matrix with minimal spectral norm, \mathbf{K}_{d^*} , has to be permutationally similar to the block-diagonal matrix with diagonal blocks of odd order as small as possible. Hence we obtain immediately case (iii) and respective form of \mathbf{K}_{d^*} for $t = 7$. For $t = 2$ and $t = 4$ such a situation is impossible. Thus, we obtain respective forms of \mathbf{K}_{d^*} . For case (iv) it is enough to observe that considered t 's can be expressed as $3i + 5j$, where $i \in \mathbb{N} \cup \{0\}, j \in \mathbb{N}$. Again from (5) and (6) condition (4) is satisfied for \mathbf{K}_{d^*} in a given form.

Let $\mathbf{K}_d \in \mathcal{K}_t \setminus \tilde{\mathcal{K}}_t$. It is known that the spectral norm of the nonnegative-definite matrix is not smaller than the maximal diagonal entry of this matrix (see e.g. Marshall and Olkin, 1979). We will show, that the maximal diagonal entry is not smaller than the upper bound of

the spectral norm of the matrix from $\tilde{\mathcal{K}}_t$ (obtained from the triangle inequality). For simplicity we denote the entries of $\mathbf{K}_d \mathbf{K}'_d$ by \tilde{k}_{ij} , $i, j = 1, 2, \dots, t$. We obtain

$$\lambda_1(\mathbf{K}_d \mathbf{K}'_d) \geq \max_i \tilde{k}_{ii}$$

and it can be observed that $\max_{1 \leq i \leq t} \tilde{k}_{ii} \geq 4$. Hence $\sigma_1(\mathbf{K}_d) \geq 2$.

Observing $\sigma_1(\mathbf{K}_{d^*}) = \sigma_1(\mathbf{P}_{d^*} - \mathbf{I}_t) \leq \sigma_1(\mathbf{P}_{d^*}) + \sigma_1(\mathbf{I}_t) = 2$ we obtain the thesis.

The second part of the theorem is obtained directly from the spectral norm of $(\mathbf{H}_3 - \mathbf{I}_3)(\mathbf{H}'_3 - \mathbf{I}_3)$ and $\mathbf{H}_5 - \mathbf{I}_5$, respectively. ■

According to the Theorem 3.1 we can formulate the following corollary, which gives the structure of the left-neighboring matrix of E-optimal design.

Corollary 3.1 *If there exists design d^* with the left-neighboring matrix \mathbf{S}_{d^*} permutationally similar to the matrix*

- (i) $\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t + \mathbf{H}_t$ for $t = 2, 7$;
- (ii) $\mathbf{1}_4 \mathbf{1}'_4 - \mathbf{I}_4 + \mathbf{I}_2 \otimes \mathbf{H}_2$ for $t = 4$;
- (iii) $\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t + \mathbf{I}_m \otimes \mathbf{H}_3$ for $t = 3m$, $m \in \mathbb{N}$;
- (iv) $\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t + \text{diag}(\mathbf{I}_i \otimes \mathbf{H}_3, \mathbf{I}_j \otimes \mathbf{H}_5)$, for $t = 5$ or $t \geq 8$ and $t \neq 3m$, $m \in \mathbb{N}$,
up to the order of diagonal blocks, where $t = 3i + 5j$ for some $i \in \mathbb{N} \cup \{0\}$ and $j \in \mathbb{N}$,

then d^* is E-optimal over $\mathcal{B}_{t,t,t}$.

Note, that in case (ii) of Corollary 3.1 there is only one form of the left-neighboring matrix, while in Theorem 3.1 there are two forms of \mathbf{K}_{d^*} . It follows from the fact, that the design with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{H}_4 - \mathbf{I}_4 + \mathbf{1}_4 \mathbf{1}'_4$ does not exist (cf. Azaïs et al., 1993).

Now we prove, that the designs with left-neighboring matrices given in Corollary 3.1 are E-optimal over the class of all designs $\mathcal{D}_{t,t,t}$. For $d \in \mathcal{D}_{t,b,k}$, the information matrix \mathbf{C}_d is of the form (3). Since \mathbf{C}_d is nonnegative-definite, the following inequality is satisfied:

$$\lambda_{t-1}(\mathbf{C}_d) \leq \lambda_{t-1}(\mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_b \otimes \mathbf{1}_k} \mathbf{T}_d). \quad (7)$$

Observe, that for $d \in \mathcal{D}_{t,b,t}$

$$\mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_t \otimes \mathbf{1}_t} \mathbf{T}_d = \mathbf{L}'_d \mathbf{Q}_{\mathbf{I}_t \otimes \mathbf{1}_t} \mathbf{L}_d = \mathbf{T}'_d \mathbf{T}_d - \frac{1}{t} \sum_{j=1}^b \mathbf{r}_{dj} \mathbf{r}'_{dj} = \mathbf{R}_d - \frac{1}{t} \sum_{j=1}^b \mathbf{r}_{dj} \mathbf{r}'_{dj}, \quad (8)$$

where \mathbf{r}_j is the t -vector of replications of treatments in the j th block and \mathbf{R}_d is the diagonal matrix with the number of replications of the i th treatment in the design on the diagonal, i.e. $\mathbf{R}_d = \text{diag}(r_{d1}, \dots, r_{dt})$. We can prove the following.

Theorem 3.2 *If design d^* satisfies conditions of Corollary 3.1, then d^* is E-optimal over $\mathcal{D}_{t,t,t}$.*

Proof. Let d^* satisfies conditions of Corollary 3.1 and let $d \in \mathcal{D}_{t,t,t} \setminus \mathcal{B}_{t,t,t}$. We prove the theorem in two steps. First we show the thesis for equireplicated designs and then for designs which are not equireplicated.

(i) If d is equireplicated, then $\mathbf{R}_d = t\mathbf{I}_t$ in (8) and

$$\lambda_{t-1}(\mathbf{T}'_d \mathbf{Q}_{I_t \otimes 1_t} \mathbf{T}_d) = t - \frac{1}{t} \lambda_{max} \left(\sum_{j=1}^t \mathbf{r}_{dj} \mathbf{r}'_{dj} \right).$$

Using the fact that the diagonal elements of a nonnegative-definite matrix are majorized by the characteristic roots, we have

$$t - \frac{1}{t} \lambda_{max} \left(\sum_{j=1}^t \mathbf{r}_{dj} \mathbf{r}'_{dj} \right) \leq t - \frac{1}{t} \max_{1 \leq i \leq t} \left(\sum_{j=1}^t r_{dij}^2 \right),$$

where r_{dij} is the number of occurrences of the i th treatment in the j th block in the design d . Since design d is not binary, we get

$$\max_{1 \leq i \leq t} \left(\sum_{j=1}^t r_{dij}^2 \right) > 4.$$

According to (7) and (5) we obtain $\lambda_{t-1}(\mathbf{C}_d) \leq t - \frac{4}{t} \leq t - \frac{1}{t} \lambda_{max}(\mathbf{K}_{d^*} \mathbf{K}'_{d^*}) = \lambda_{t-1}(\mathbf{C}_{d^*})$.

(ii) If d is not equireplicated, then minimal diagonal element in \mathbf{R}_d given in (8) is not greater than $t - 1$. From Constantine (1981)

$$\lambda_{t-1}(\mathbf{T}'_d \mathbf{Q}_{I_t \otimes 1_t} \mathbf{T}_d) \leq \frac{(k-1)t}{k(t-1)} \min_{1 \leq i \leq t} r_{di}, \quad (9)$$

and thus in our case

$$\lambda_{t-1}(\mathbf{C}_d) \leq \min_{1 \leq i \leq t} r_{di} \leq t - 1 \leq t - \frac{4}{t} \leq \lambda_{t-1}(\mathbf{C}_{d^*})$$

for $t \geq 4$. For $t = 2, 3$ the thesis is obtained by direct calculations. ■

4 E-optimal designs over $\mathcal{D}_{t,t-2,t}$

In this section we determine the structure of the left-neighboring matrix of E-optimal design over $\mathcal{D}_{t,t-2,t}$. Similarly as in previous section first we determine, which structure of \mathbf{K}_d from $\widehat{\mathcal{K}}_{t-2}$ gives the minimal spectral norm over \mathcal{K}_{t-2} . Then we show the structure of the left-neighboring matrix of E-optimal design over the class of binary designs $\mathcal{B}_{t,t-2,t}$ and, finally, over the class of all designs $\mathcal{D}_{t,t-2,t}$.

Theorem 4.1 *The matrix \mathbf{K}_{d^*} which minimizes the spectral norm over \mathcal{K}_{t-2} is permutationally similar to the matrix $\frac{2}{t}\mathbf{1}_t\mathbf{1}'_t - \mathbf{I}_t - \mathbf{H}_t$.*

Proof.

Let $\mathbf{K}_d \in \widehat{\mathcal{K}}_{t-2}$. Then $\mathbf{K}_d\mathbf{K}'_d = 2\mathbf{I}_t - \frac{4}{t}\mathbf{1}_t\mathbf{1}'_t + (\mathbf{P}_d + \mathbf{P}'_d)$, $\mathbf{P}_d \in \overline{\mathcal{P}}_t$. Observe, that for $\mathbf{P}_{d^*} = \mathbf{H}_t$ the unordered eigenvalues of $\mathbf{K}_{d^*}\mathbf{K}'_{d^*}$ are of the form

$$\mu_i(\mathbf{K}_{d^*}\mathbf{K}'_{d^*}) = \begin{cases} 0 & \text{for } i = 0 \\ 2 + 2 \cos \frac{2i\pi}{t} & \text{for } i = 1, 2, \dots, t-1 \end{cases}$$

and we obtain the maximal eigenvalue of $\mathbf{K}_{d^*}\mathbf{K}'_{d^*}$ for $i = 1$ or $i = t-1$, i.e.

$$\lambda_{\max}(\mathbf{K}_{d^*}\mathbf{K}'_{d^*}) = 2 + 2 \cos \frac{2\pi}{t} = 4 \cos^2 \frac{\pi}{t}. \quad (10)$$

Let $\mathbf{P}_d = \text{diag}(\mathbf{H}_{t_1}, \dots, \mathbf{H}_{t_n})$, $t_1 + \dots + t_n = t$. Then the unordered, nonzero eigenvalues of $\mathbf{K}_d\mathbf{K}'_d$ are

$$\mu_m(\mathbf{K}_d\mathbf{K}'_d) = 2 + 2 \cos \frac{2i\pi}{t_j} \quad \text{for } \begin{matrix} m = 1, 2, \dots, t-1, \\ i = 1, 2, \dots, t_1-1, 0, 1, \dots, t_2-1, \dots, 0, 1, \dots, t_n-1, \\ j = 1, \dots, n, \end{matrix}$$

and we get $\lambda_{\max}(\mathbf{K}_d\mathbf{K}'_d)$ for $i = 0$ and finally

$$\lambda_{\max}(\mathbf{K}_d\mathbf{K}'_d) = 4 > 4 \cos^2 \frac{\pi}{t} = \lambda_{\max}(\mathbf{K}_{d^*}\mathbf{K}'_{d^*}).$$

Let $\mathbf{K}_d \in \mathcal{K}_{t-2} \setminus \widehat{\mathcal{K}}_{t-2}$. It is known, that the spectral norm of a matrix is not smaller than the spectral norm of any submatrix of this matrix (cf. Horn and Johnson, 1991). We use a 2×2 submatrix of $\mathbf{K}_d\mathbf{K}'_d$.

Observe, that in the class $\mathcal{K}_{t-2} \setminus \widehat{\mathcal{K}}_{t-2}$ the matrix \mathbf{K}_d has at least two entries equals to $2 - \frac{t-2}{t}$, and these two entries are in different rows, say in positions (i_1, j_1) and (i_2, j_2) , $i_1 \neq i_2$, $j_1 \neq j_2$ (it follows from zero row and column sum of \mathbf{K}_d). In such a situation two diagonal entries of $\mathbf{K}_d\mathbf{K}'_d$ are equal to $4 - \frac{4}{t}$ and the (i_1, j_2) th entry of $\mathbf{K}_d\mathbf{K}'_d$ is equal to $-\frac{4}{t}$ or $1 - \frac{4}{t}$ or $3 - \frac{4}{t}$. Let \mathbf{A} be the symmetric submatrix of $\mathbf{K}_d\mathbf{K}'_d$ of order 2, which contains entries (i_1, j_1) and (i_2, j_2) on the diagonal and (i_1, j_2) as off-diagonal entries. Then

$$\sigma_1(\mathbf{K}_d) \geq \sqrt{\lambda_{\max}(\mathbf{A})} = \begin{cases} \sqrt{3} & \text{for } t = 2, 3, 4, \\ \sqrt{5 - \frac{8}{t}} & \text{for } t = 5, 6, 7, \\ 2 & \text{for } t \geq 8. \end{cases}$$

It is easy to calculate that the above spectral norm of \mathbf{K}_d is not smaller than the spectral norm $\sigma_1(\mathbf{K}_{d^*}) = 2 \cos \frac{\pi}{t}$ obtained from (10). The proof is complete. \blacksquare

Corollary 4.1 *If there exists design d^* with the left-neighboring matrix \mathbf{S}_{d^*} permutationally similar to the matrix $\mathbf{1}_t\mathbf{1}'_t - \mathbf{I}_t - \mathbf{H}_t$, then d^* is E-optimal over $\mathcal{B}_{t,t-2,t}$.*

Now we prove, that the designs with left-neighboring matrices given in the above corollary are E-optimal over the class of all designs $\mathcal{D}_{t,t-2,t}$.

Theorem 4.2 *If design d^* satisfies conditions of Corollary 4.1, then d^* is E-optimal over $\mathcal{D}_{t,t-2,t}$.*

Proof. Let d^* be an E-optimal design over $\mathcal{B}_{t,t-2,t}$ and let $d \in \mathcal{D}_{t,t-2,t} \setminus \mathcal{B}_{t,t-2,t}$. We prove the theorem in two steps. First we consider equireplicated designs and in second step we study the class of not equireplicated designs.

(i) If d is equireplicated, then $\mathbf{R}_d = (t-2)\mathbf{I}_t$ in (8) and

$$\lambda_{t-1}(\mathbf{T}'_d \mathbf{Q}_{\mathbf{I}_t \otimes \mathbf{1}_t} \mathbf{T}_d) = t - 2 - \frac{1}{t} \lambda_{\max} \left(\sum_{j=1}^{t-2} \mathbf{r}_{dj} \mathbf{r}'_{dj} \right).$$

Using the fact that the diagonal elements of a nonnegative-definite matrix are majorized by the characteristic roots, we get

$$t - 2 - \frac{1}{t} \lambda_{\max} \left(\sum_{j=1}^{t-2} \mathbf{r}_{dj} \mathbf{r}'_{dj} \right) \leq t - 2 - \frac{1}{t} \max_{1 \leq i \leq t} \left(\sum_{j=1}^{t-2} r_{dij}^2 \right),$$

where r_{dij} is the number of occurrences of the i th treatment in the j th block in the design d . Since design d is not binary, we obtain

$$\max_{1 \leq i \leq t} \left(\sum_{j=1}^{t-2} r_{dij}^2 \right) > 4 + t - 4 = t.$$

According to (7) and (10) we have

$$\lambda_{t-1}(\mathbf{C}_d) \leq t - 3 \leq t - 2 - \frac{1}{t-2} \cdot 4 \cos^2 \frac{\pi}{t} = \lambda_{t-1}(\mathbf{C}_{d^*}).$$

(ii) If d is not equireplicated, then minimal diagonal element in \mathbf{R}_d given in (8) is not greater than $t - 3$. Using (9) we obtain

$$\lambda_{t-1}(\mathbf{C}_d) \leq \min_{1 \leq i \leq t} r_{di} \leq t - 3 \leq t - 2 - \frac{1}{t-2} \cdot 4 \cos^2 \frac{\pi}{t} = \lambda_{t-1}(\mathbf{C}_{d^*}).$$

■

5 Construction of E-optimal designs

In accordance to Corollary 3.1 and 4.1 we can identify the left-neighboring matrix \mathbf{S}_{d^*} of an E-optimal design. In this section we give the method of construction of E-optimal designs over $\mathcal{D}_{t,t,t}$ and $\mathcal{D}_{t,t-2,t}$.

From the form of the matrix \mathbf{T}_d we can observe that each block of complete binary design can be written as a one-cycle permutation matrix. Thus, if we decompose the left-neighboring matrix to the sum of b one-cycle permutation matrices, we can construct a design. Recall, that each permutation is a cycle or a product of disjoint cycles (see e.g. Birkhoff and Mac Lane, 1954). For example, the matrix \mathbf{H}'_3 is a one-cycle permutation matrix, which presents the cycle: $1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 1$ (indexes of elements of \mathbf{H}'_3 that equal 1). Observe that, if we write this cycle in the form [123], we can regard it as a treatment sequence in a single block of design.

Consider the class $\mathcal{D}_{t,t,t}$. From Corollary 3.1. it follows that the left-neighboring matrix of an E-optimal design has zero diagonal, exactly one off-diagonal element equal to 2 in each row and column, and the remaining off-diagonal elements are equal to 1. This implies that an E-optimal design has two classes of ordered pairs of neighboring treatments: $t(t-2)$ pairs which occur exactly once in a design and t ordered pairs which occur exactly twice in a design. The main problem in the construction of E-optimal designs is determining which pairs occur once in a design and which twice.

Since for different t we have different forms of \mathbf{S}_{d^*} , the methods of construction of E-optimal designs are different.

Observe that the left-neighboring matrix of circular neighbor balanced design (CNBD), \mathbf{S}_{CNBD} , is of the form $\mathbf{S}_{\text{CNBD}} = \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t$. From Corollary 3.1 it can be noticed that for $t = 3, 5, 7$ the matrix \mathbf{S}_{d^*} is obtained by adding one-cycle permutation matrix to \mathbf{S}_{CNBD} . Thus, in such a case E-optimal designs can be constructed from CNBD by repeating one arbitrary block.

Example. Let $t = 3, 5$ or 7 . The following designs are E-optimal over $\mathcal{D}_{t,t,t}$:

for $t = 3$:

$$d^* = \begin{pmatrix} 1 & 3 & 2 \\ 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix},$$

for $t = 5$:

$$d^* = \begin{pmatrix} 1 & 5 & 4 & 3 & 2 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \\ 1 & 4 & 2 & 5 & 3 \\ 1 & 5 & 4 & 3 & 2 \end{pmatrix},$$

for $t = 7$:

$$d^* = \begin{pmatrix} 1 & 7 & 6 & 5 & 4 & 3 & 2 \\ 1 & 6 & 4 & 2 & 7 & 5 & 3 \\ 1 & 5 & 2 & 6 & 3 & 7 & 4 \\ 1 & 4 & 7 & 3 & 6 & 2 & 5 \\ 1 & 3 & 5 & 7 & 2 & 4 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 7 & 6 & 5 & 4 & 3 & 2 \end{pmatrix}.$$

For the remaining t observe, that if we express \mathbf{S}_{d^*} as the sum $\mathbf{S}_{\text{CNBD}} + \mathbf{P}_t$, then \mathbf{P}_t is not one-cycle permutation matrix (\mathbf{P}_t can not be the left-neighboring matrix of any block of a design). Thus, E-optimal designs can not to be constructed from CNBD. Some hints how to construct such designs (how to decompose \mathbf{S}_{d^*}) are given in Filipiak and Rózański, 2005. In this paper we give only some examples.

Example. The following designs are E-optimal over $\mathcal{D}_{t,t,t}$:

for $t = 4$:

$$d^* = \begin{pmatrix} 1 & 4 & 3 & 2 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 4 & 3 \\ 1 & 3 & 4 & 2 \end{pmatrix},$$

for $t = 6$:

$$d^* = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 4 & 6 & 5 & 3 \\ 1 & 3 & 2 & 5 & 6 & 4 \\ 1 & 4 & 5 & 2 & 6 & 3 \\ 1 & 5 & 4 & 3 & 6 & 2 \\ 1 & 6 & 4 & 2 & 3 & 5 \end{pmatrix},$$

for $t = 8$:

$$d^* = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 2 & 4 & 6 & 8 & 7 & 5 & 3 \\ 1 & 3 & 2 & 5 & 4 & 7 & 8 & 6 \\ 1 & 4 & 2 & 3 & 8 & 5 & 6 & 7 \\ 1 & 5 & 7 & 4 & 8 & 2 & 6 & 3 \\ 1 & 6 & 2 & 7 & 3 & 5 & 8 & 4 \\ 1 & 7 & 2 & 8 & 3 & 6 & 4 & 5 \\ 1 & 8 & 4 & 3 & 7 & 6 & 5 & 2 \end{pmatrix}.$$

Consider the class $\mathcal{D}_{t,t-2,t}$. Let design d^* has the left-neighboring matrix \mathbf{S}_{d^*} given in Corollary 4.1. Observe, that the matrix $\mathbf{1}_t \mathbf{1}_t' - \mathbf{I}_t$ in \mathbf{S}_{d^*} is the left-neighboring matrix of circular neighbor balanced design (CNBD). Thus, subtracting a matrix permutationally similar to \mathbf{H}_t (which is full-cycle permutation matrix) is equivalent to abridging one arbitrary block from CNBD. Thus, design d^* can be construct from CNBD by abridging one arbitrary block. the cataogue of CNBDs can be found in Azaïs et al., 1993.

Example. The following designs are E-optimal over $\mathcal{D}_{t,t-2,t}$:

for $t = 5$:

$$d^* = \begin{pmatrix} 1 & 5 & 4 & 3 & 2 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \end{pmatrix},$$

for $t = 8$:

$$d^* = \begin{pmatrix} 1 & 2 & 6 & 3 & 5 & 4 & 8 & 7 \\ 1 & 4 & 6 & 5 & 8 & 2 & 7 & 3 \\ 1 & 7 & 6 & 8 & 3 & 4 & 2 & 5 \\ 1 & 8 & 4 & 7 & 5 & 3 & 6 & 2 \\ 1 & 3 & 2 & 8 & 5 & 6 & 7 & 4 \\ 1 & 5 & 7 & 2 & 4 & 3 & 8 & 6 \end{pmatrix}.$$

Acknowledgements

The authors are thankful to Professor Charles R. Johnson for helpful discussion on the topic of this paper during the conference MAT-TRIAD 2005.

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