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On the Optimality of Circular Block Designs Under a Mixed Interference Model

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Filipiak and Markiewicz (2012) proved the universal optimality of circular weakly neighbor balanced designs (CWNBDs) under the interference model with fixed neighbor effects among the class of complete block designs. In two special cases where a CWNBD cannot exist, Filipiak et al. (2012) characterized D-optimal designs. The aim of this paper is to show the universal optimality of CWNBDs and to characterize D-optimal designs under the interference model with random neighbor effects.

Keywords Circular weakly neighbor balanced designs; D-optimality; Information matrix; Interference model; Left-neighboring matrix; Universal optimality.

Mathematics Subject Classification 62K05; 62K10.

1. Introduction

A basic problem in the theory of experimental designs is to characterize optimal designs. If in an experiment the response to a treatment is affected by the other treatments (for example, in agricultural and horticultural experiments), then the optimality of designs under an interference model is studied. David et al. (2001) use several models to analyze data from such trials, including a model with random interference effects. Jones et al. (1992) give information matrices for a mixed effects model with random interference effects with the same variances and determine optimal repeated measurements designs. Filipiak and Markiewicz (2003, 2007) proved the universal optimality of circular neighbor balanced designs (CNBDs) under an interference model with random neighbor effects. This is an extension of results presented by Druilhet (1999) for a fixed interference model. Filipiak and Markiewicz (2012) showed that circular weakly neighbor balanced designs (CWNBDs) are universally optimal under the fixed interference model. The aim of this paper is to generalize these results for the mixed interference model with random neighbor effects.

The conditions for the existence of CNBDs and CWNBDs are quite strict: see, for example, Druilhet (1999) and Filipiak and Markiewicz (2012). In the case where the

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universally optimal designs cannot exist, optimality with respect to the specified criteria is considered. Filipiak et al. (2008) and Filipiak et al. (2012) characterized E- and D-optimal designs under the fixed interference models over some classes of complete block designs with t treatments and $b = t - 2$ or $b = t$. It is interesting to extend these results to the mixed interference model. The problem of the characterization of E-optimal complete block designs is considered in Filipiak and Róžański (2012). The aim of this paper is to characterize D-optimal designs among some complete block designs under the mixed interference model.

This paper is organized as follows. First we present some general definitions and notation. In Sec. 3 we prove the universal optimality of CWNBDs over the class of equireplicated complete block designs. In Sec. 4 we characterize the structure of the left-neighboring matrix of a D-optimal design with $t = k = b + 2$ and $t = k = b$, and we make some remarks on the construction of D-optimal designs with examples. In both sections we assume the mixed interference model.

2. Definitions and Notation

Let us consider an experiment in which t treatments are arranged in n non-homogeneous units grouped in b blocks each of size k . The set of such designs we denote by $\mathcal{D}_{t,b,k}$. An interference model with left-neighbor effects associated with the design $d \in \mathcal{D}_{t,b,k}$ can be written as

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

where $\boldsymbol{\tau}$ and $\boldsymbol{\beta}$ are the vectors of treatment and block effects, respectively. Here $\boldsymbol{\lambda}$ and $\boldsymbol{\varepsilon}$ are the vectors of random left-neighbor effects and random errors, respectively, with $E(\boldsymbol{\lambda}) = \mathbf{0}_t$, $\text{Cov}(\boldsymbol{\lambda}) = \sigma_L^2 \mathbf{I}_t$, $E(\boldsymbol{\varepsilon}) = \mathbf{0}_n$, $\text{Cov}(\boldsymbol{\varepsilon}) = \mathbf{I}_n$, and $\text{Cov}(\boldsymbol{\lambda}, \boldsymbol{\varepsilon}) = \mathbf{0}_n$, where σ_L^2 is a known constant. The matrices \mathbf{I}_n and $\mathbf{0}_n$ are identity and zero matrices of order n , respectively, and $\mathbf{0}_n$ is n -dimensional vector of zeros. The matrix $\mathbf{B} = \mathbf{I}_b \otimes \mathbf{1}_k$ is the design matrix of block effects, where $\mathbf{1}_k$ is a k -dimensional vector of ones and \otimes denotes the Kronecker product. By $\boldsymbol{\Sigma}$ we denote $\text{Cov}(\mathbf{y}) = \sigma_L^2 \mathbf{L}_d \mathbf{L}_d' + \mathbf{I}_{bk}$.

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:

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

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). The border plots receive treatments but are not used for measuring the response variables.

Model (1) with random neighbor effects $\boldsymbol{\lambda}$ is called a *mixed interference model* and is denoted by \mathcal{M}_σ . Following Jones et al. (1992), by \mathcal{M}_∞ we denote the model in which the variance tends to infinity ($\sigma_L^2 = \infty$). Such a model is called a *fixed interference model*. On

the other hand, if $\sigma_L^2 = 0$, model (1) is a model without neighbor effects and is denoted by \mathcal{M}_0 .

For any $m \times n$ matrix \mathbf{A} we define $\mathbf{Q}_A = \mathbf{I}_m - \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'$, the orthogonal projector on the orthocomplement of the column span of a matrix \mathbf{A} , where $(\mathbf{A}'\mathbf{A})^{-}$ denotes a generalized inverse of $\mathbf{A}'\mathbf{A}$. Observe that $\mathbf{Q}_B = \mathbf{I}_b \otimes \mathbf{E}_k$, where $\mathbf{E}_k = \mathbf{I}_k - \frac{1}{k}\mathbf{1}_k\mathbf{1}'_k$.

Further, let $\mathbf{C}_{d,u}$ denote information matrices of d for estimating $\boldsymbol{\tau}$ in model \mathcal{M}_u under normality, where $u \in \{\sigma, \infty\}$.

From Filipiak and Markiewicz (2007), for $\text{Cov}(\boldsymbol{\lambda}) = \sigma_L^2\mathbf{I}_t$ the information matrix $\mathbf{C}_{d,\sigma}$ can be expressed as

$$\mathbf{C}_{d,\sigma} = \mathbf{T}'_d\mathbf{Q}_B\mathbf{T}_d - \sigma_L^2\mathbf{T}'_d\mathbf{Q}_B\mathbf{L}_d(\sigma_L^2\mathbf{L}'_d\mathbf{Q}_B\mathbf{L}_d + \mathbf{I}_t)^{-1}\mathbf{L}'_d\mathbf{Q}_B\mathbf{T}_d \quad (2)$$

or equivalently, from Jones et al. (1992), as

$$\mathbf{C}_{d,\sigma} = \mathbf{T}'_d\boldsymbol{\Sigma}^{-1}\mathbf{T}_d - \mathbf{T}'_d\boldsymbol{\Sigma}^{-1}\mathbf{B}(\mathbf{B}'\boldsymbol{\Sigma}^{-1}\mathbf{B})^{-1}\mathbf{B}'\boldsymbol{\Sigma}^{-1}\mathbf{T}_d = \mathbf{T}'_d\boldsymbol{\Sigma}^{-1/2}\mathbf{Q}_{\boldsymbol{\Sigma}^{-1/2}\mathbf{B}}\boldsymbol{\Sigma}^{-1/2}\mathbf{T}_d \quad (3)$$

with $\boldsymbol{\Sigma}^{-1} = \mathbf{I}_n - \mathbf{L}_d\boldsymbol{\Lambda}\mathbf{L}'_d$, where $\boldsymbol{\Lambda}$ is a diagonal matrix of order t with $\frac{\sigma_L^2}{1+r_i\sigma_L^2}$, $i = 1, \dots, t$, and r_i is the number of replications of the i th treatment in the design.

Since $\mathbf{1}_n$ is a vector in the column span of matrix \mathbf{B} , the following inequality is satisfied:

$$\mathbf{C}_{d,\sigma} = \mathbf{T}'_d\boldsymbol{\Sigma}^{-1/2}\mathbf{Q}_{\boldsymbol{\Sigma}^{-1/2}\mathbf{B}}\boldsymbol{\Sigma}^{-1/2}\mathbf{T}_d \leq_L \mathbf{T}'_d\boldsymbol{\Sigma}^{-1/2}\mathbf{Q}_{\boldsymbol{\Sigma}^{-1/2}\mathbf{1}_n}\boldsymbol{\Sigma}^{-1/2}\mathbf{T}_d, \quad (4)$$

for every design $d \in \mathcal{D}_{t,b,k}$, where for two $t \times t$ symmetric matrices \mathbf{A} and \mathbf{B} the notation $\mathbf{A} \leq_L \mathbf{B}$ means that \mathbf{A} is below \mathbf{B} in the Loewner ordering, i.e., $\mathbf{B} - \mathbf{A}$ is non-negative definite. The matrix on the right-hand side of (4) is the information matrix for the interference model with general mean and random neighbor effects and without block effects, i.e.,

$$\mathbf{y} = \mu\mathbf{1}_n + \mathbf{T}_d\boldsymbol{\tau} + \mathbf{L}_d\boldsymbol{\lambda} + \boldsymbol{\varepsilon}, \quad (5)$$

with $\text{Cov}(\mathbf{y}) = \sigma_L^2\mathbf{L}_d\mathbf{L}'_d + \mathbf{I}_{bk}$. Such a model can be studied if the experiment is assumed to use circular blocks, but the experimental conditions may be equal in every block; cf. Hwang (1973).

It should be noted that from the equality $\mathbf{H}'_k\mathbf{E}_k\mathbf{H}_k = \mathbf{E}_k$ it follows that $\mathbf{L}'_d\mathbf{Q}_B\mathbf{L}_d = \mathbf{T}'_d\mathbf{Q}_B\mathbf{T}_d$. Moreover, since the matrix $\mathbf{Q}_B\mathbf{T}_d$ has zero row sums, the matrices $\mathbf{T}'_d\mathbf{Q}_B\mathbf{T}_d$, $\mathbf{T}'_d\mathbf{Q}_B\mathbf{L}_d$ in (2) and $\mathbf{C}_{d,\sigma}$ have row and column sums zero. Observe that

$$\mathbf{T}'_d\mathbf{Q}_B\mathbf{L}_d = \mathbf{T}'_d\mathbf{L}_d - k^{-1}\mathbf{T}'_d\mathbf{B}\mathbf{B}'\mathbf{L}_d = \mathbf{S}_d - k^{-1}\mathbf{N}_d\mathbf{N}'_d,$$

where $\mathbf{S}_d = \mathbf{T}'_d\mathbf{L}_d = (s_{d,ij})_{1 \leq i,j \leq t}$ is called a *left-neighboring matrix* of design d (c.f. Filipiak et al., 2008) and $\mathbf{N}_d = \mathbf{B}'\mathbf{T}_d = \mathbf{B}'\mathbf{L}_d = (n_{d,ij})_{1 \leq i \leq t, 1 \leq j \leq b}$ is an incidence matrix of design d . For a design $d \in \mathcal{D}_{t,b,k}$ the symbols $s_{d,ij}$ and $n_{d,ij}$ are, respectively, the number of occurrences of treatment i with treatment j as a left neighbor and the number of occurrences of treatment i in block j . It is easy to see that $\mathbf{S}_d\mathbf{1}_t = \mathbf{r}_d$, where $\mathbf{r}_d = (\mathbf{r}_{di})_{1 \leq i \leq t}$ is a vector of replications of treatments. Moreover, for binary complete block designs, i.e., designs with $t = k$ such that every treatment occurs once in each block, $\mathbf{N}_d = \mathbf{1}_t\mathbf{1}'_b$ and the information matrix $\mathbf{C}_{d,\sigma}$ depends on the design only with respect to \mathbf{S}_d .

Since the matrix $\mathbf{C}_{d,\sigma}$ has zero row and column sums, to characterize universally optimal designs we use Kiefer's (1975) Proposition 1.

Assume that we have a design $d^* \in \mathcal{D}_{t,b,k}$ such that $\mathbf{C}_{d^*,u}$, $u \in \{\sigma, \infty\}$ is completely symmetric and that $\text{tr}\mathbf{C}_{d^*,u}$ is maximal over $\mathcal{D}_{t,b,k}$. Then the design d^* is universally optimal in Kiefer's sense in the class $\mathcal{D}_{t,b,k}$ under the model \mathcal{M}_u .

Recall that an $m \times m$ matrix \mathbf{A} is called *completely symmetric* if all its diagonal elements are equal and all its off-diagonal elements are equal.

It is known that for some combinations of design parameters, for example, $t = k = b+2$ or $t = k = b$, universally optimal designs cannot exist (for more details see, e.g., Druilhet, 1999, Filipiak and Markiewicz, 2003, 2007, 2012). Therefore in such cases we characterize D-optimal designs over some special classes of designs under the mixed interference model. The presented results are an extension of results given by Filipiak et al. (2012) for the fixed interference model.

A design $d^* \in \mathcal{D}_{t,b,k}$ is called *D-optimal* over $\mathcal{D}_{t,b,k}$ if $\prod_{i=1}^{t-1} \lambda_i(\mathbf{C}_{d^*,u}) \geq \prod_{i=1}^{t-1} \lambda_i(\mathbf{C}_{d,u})$, $u \in \{\sigma, \infty\}$, for all designs $d \in \mathcal{D}_{t,b,k}$, where $0 = \lambda_0(\mathbf{C}_{d,u}) \leq \lambda_1(\mathbf{C}_{d,u}) \leq \dots \leq \lambda_{t-1}(\mathbf{C}_{d,u})$ are the eigenvalues of the information matrix $\mathbf{C}_{d,u}$; cf. Pukelsheim (1993).

Throughout the paper we will use the property of permutational similarity. Recall, that the matrix $\mathbf{P}'\mathbf{A}\mathbf{P}$, where $\mathbf{P} \in \mathcal{P}_t$ is a permutation matrix of order t and \mathbf{A} is an arbitrary $t \times t$ matrix, is said to be *permutationally similar* to \mathbf{A} . It is known that the eigenvalues (and consequently the determinant) of \mathbf{A} and a matrix permutationally similar to \mathbf{A} are equal.

3. Universal Optimality of Designs

Let us define CWNBDS as follows.

Definition 1. (Filipiak and Markiewicz, 2012)

Let $b \neq x(t-1)$, $x \in \mathbb{N}$. A circular binary design $d \in \mathcal{D}_{t,b,t}$ with $s_{d,ij} \in \{x-1, x\}$, $i \neq j$, and completely symmetric matrix $\mathbf{S}_d \mathbf{S}'_d$ is called a CWNBD.

Note that for $b = x(t-1)$ we obtain the definition of CNBD, i.e., a design with $\mathbf{S}_d = x(\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t)$; cf. Druilhet (1999).

From Filipiak and Markiewicz (2012) it follows that a necessary condition for the existence of a CWNBD with $(x-1)(t-1) < b \leq x(t-1)$, $x \in \mathbb{N}$ is

$$\frac{b(b-2x+1)}{t-1} \in \mathbb{N}.$$

Filipiak and Markiewicz (2012) proved the universal optimality of CWNBDS under the model \mathcal{M}_∞ among the designs from $\mathcal{D}_{t,b,t}$ if $b \leq t-1$, and from $\overline{\mathcal{R}}_{t,b,t}$ if $b > t-1$, where $\overline{\mathcal{R}}_{t,b,k} \subset \mathcal{D}_{t,b,k}$ is the class of equireplicated designs with no treatment preceded by itself. In this section, we study the universal optimality of CWNBDS under the model \mathcal{M}_σ . By $\mathcal{R}_{t,b,k} \subset \mathcal{D}_{t,b,k}$ we denote the class of equireplicated designs.

Theorem 1. For every $\sigma_L^2 \in (0, \infty]$ a CWNBD is universally optimal over the class $\mathcal{R}_{t,b,t}$, $b < t-1$, and over the class $\overline{\mathcal{R}}_{t,b,t}$, $b > t-1$, under the interference model \mathcal{M}_σ .

Proof. Let $d^* \in \mathcal{D}_{t,b,t}$ be a CWNBD such that $(x-1)(t-1) < b \leq x(t-1)$, $x \in \mathbb{N}$. Since CWNBD is binary and complete, $\mathbf{T}'_{d^*} \mathbf{B} = \mathbf{1}_t \mathbf{1}'_b$, $\mathbf{\Sigma}^{-1} = \mathbf{I}_{bk} - \frac{\sigma_L^2}{1+b\sigma_L^2} \mathbf{L}_{d^*} \mathbf{L}'_{d^*}$ and

$$\begin{aligned} \mathbf{T}'_{d^*} \mathbf{\Sigma}^{-1} \mathbf{T}_{d^*} &= b\mathbf{I}_t - \frac{\sigma_L^2}{1+b\sigma_L^2} \mathbf{S}_{d^*} \mathbf{S}'_{d^*}, & \mathbf{T}'_{d^*} \mathbf{\Sigma}^{-1} \mathbf{B} &= \frac{1}{1+b\sigma_L^2} \mathbf{1}_t \mathbf{1}'_b, \\ \mathbf{B}' \mathbf{\Sigma}^{-1} \mathbf{B} &= t \left(\mathbf{I}_b - \frac{\sigma_L^2}{1+b\sigma_L^2} \mathbf{1}_b \mathbf{1}'_b \right), & (\mathbf{B}' \mathbf{\Sigma}^{-1} \mathbf{B})^{-1} &= \frac{1}{t} (\mathbf{I}_b + \sigma_L^2 \mathbf{1}_b \mathbf{1}'_b) \end{aligned}$$

are the elements of (3). Hence

$$\mathbf{C}_{d^*,\sigma} = b\mathbf{I}_t - \frac{\sigma_L^2}{1 + b\sigma_L^2} \mathbf{S}_{d^*} \mathbf{S}'_{d^*} - \frac{b}{t(1 + b\sigma_L^2)} \mathbf{1}_t \mathbf{1}'_t. \quad (6)$$

Observe that all diagonal entries of \mathbf{S}_{d^*} are equal to zero, and in each row $(b - (x - 1)(t - 1))$ entries are equal to x and $(x(t - 1) - b)$ entries are equal to $x - 1$. Thus, for $i = 1, \dots, t$

$$\begin{aligned} (\mathbf{S}_{d^*} \mathbf{S}'_{d^*})_{ii} &= (b - (x - 1)(t - 1))x^2 + (x(t - 1) - b)(x - 1)^2 = \\ &= b(2x - 1) - x(x - 1)(t - 1) \end{aligned}$$

and

$$\begin{aligned} \text{tr } \mathbf{C}_{d^*,\sigma} &= bt - \frac{b}{1 + b\sigma_L^2} - \frac{\sigma_L^2}{1 + b\sigma_L^2} \text{tr } \mathbf{S}_{d^*} \mathbf{S}'_{d^*} = \\ &= bt - \frac{b}{1 + b\sigma_L^2} - \frac{t\sigma_L^2}{1 + b\sigma_L^2} (b(2x - 1) - x(x - 1)(t - 1)). \end{aligned}$$

Let $d \in \mathcal{R}_{t,b,t}$. Then

$$\mathbf{T}'_d \boldsymbol{\Sigma}^{-1} \mathbf{T}_d = b\mathbf{I}_t - \frac{\sigma_L^2}{1 + b\sigma_L^2} \mathbf{S}_d \mathbf{S}'_d, \quad \mathbf{T}'_d \boldsymbol{\Sigma}^{-1} \mathbf{1}_n = \frac{b}{1 + b\sigma_L^2} \mathbf{1}_t, \quad \mathbf{1}'_n \boldsymbol{\Sigma}^{-1} \mathbf{1}_n = \frac{bt}{1 + b\sigma_L^2}$$

and from (4)

$$\mathbf{C}_{d,\sigma} \leq_L b\mathbf{I}_t - \frac{\sigma_L^2}{1 + b\sigma_L^2} \mathbf{S}_d \mathbf{S}'_d - \frac{b}{t(1 + b\sigma_L^2)} \mathbf{1}_t \mathbf{1}'_t. \quad (7)$$

We obtain

$$\text{tr } \mathbf{C}_{d,\sigma} \leq bt - \frac{b}{1 + b\sigma_L^2} - \frac{\sigma_L^2}{1 + b\sigma_L^2} \text{tr } \mathbf{S}_d \mathbf{S}'_d$$

and it is enough to show

$$\text{tr } \mathbf{S}_d \mathbf{S}'_d \geq \text{tr } \mathbf{S}_{d^*} \mathbf{S}'_{d^*}. \quad (8)$$

(a) Let $b < t - 1$. Then

$$\text{tr } \mathbf{S}_d \mathbf{S}'_d = \sum_{i=1}^t \sum_{j=1}^t s_{d,ij}^2 \geq \sum_{i=1}^t \sum_{j=1}^t s_{d,ij} = bt = \text{tr } \mathbf{S}_{d^*} \mathbf{S}'_{d^*}.$$

(b) Let $b > t - 1$ and let $\mathbf{u} = (x, \dots, x, x - 1, \dots, x - 1)'$ be the $t(t - 1)$ -dimensional vector of integers with $\sum_{i=1}^{t(t-1)} u_i = bt$. Observe that \mathbf{u} is majorized by any other vector of integers \mathbf{v} with $\mathbf{v}' \mathbf{1}_{t(t-1)} = bt$, i.e., $\text{vec } \mathbf{S}_{d^*}$ is majorized by $\text{vec } \mathbf{S}_d$ for all $d \in \overline{\mathcal{R}}_{t,b,t}$, $b > t - 1$, where $\text{vec } \mathbf{S}_d$ denotes the vector formed by writing the columns of \mathbf{S}_d one under the other in sequence. Thus due to Proposition C.1. of Marshall and Olkin (1979, p. 64), we obtain (8). \square

Remark. A CWNBD is binary and complete, so it is balanced with respect to the blocks. Such designs are universally optimal over $\mathcal{D}_{t,b,t}$ under the model \mathcal{M}_0 ; see, e.g., Shah and Sinha (1989).

A method of construction of some CWNBDs is given in Filipiak and Markiewicz (2012).

Example 1. The following CWNBD is universally optimal over $\mathcal{R}_{7,3,7}$:

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

Now we show an example of a non-equireplicated design $d^\#$ such that

$$\text{tr} (\mathbf{T}'_{d^\#} \Sigma^{-1/2} \mathbf{Q}_{\Sigma^{-1/2} \mathbf{1}_n} \Sigma^{-1/2} \mathbf{T}_{d^\#}) > \text{tr} \mathbf{C}_{d^*, \sigma},$$

where d^* is CWNBD. This example shows that inequality (4) does not give a good upper bound for the trace of the information matrix.

Example 2. For the following design:

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

and d^* from Example 1 we have

$$\text{tr} (\mathbf{T}'_{d^\#} \Sigma^{-1/2} \mathbf{Q}_{\Sigma^{-1/2} \mathbf{1}_n} \Sigma^{-1/2} \mathbf{T}_{d^\#}) - \text{tr} \mathbf{C}_{d^*, \sigma} = \frac{2(-1 - 4\sigma_L^2 + 9\sigma_L^4)}{21 + 187\sigma_L^2 + 540\sigma_L^4 + 504\sigma_L^6}$$

which is positive for every $\sigma_L^2 > \frac{2+\sqrt{13}}{9}$. However

$$\text{tr} \mathbf{C}_{d^\#, \sigma} - \text{tr} \mathbf{C}_{d^*, \sigma} = -\frac{2(1 + 8\sigma_L^2 + 19\sigma_L^4 + 24\sigma_L^6)}{7 + 61\sigma_L^2 + 172\sigma_L^4 + 156\sigma_L^6}$$

is negative for every σ_L^2 and $d^\#$ is not better than d^* .

We should note that the above results are not surprising. Kunert (1994) considered a model

$$\mathbf{y} = \mu \mathbf{1}_n + \mathbf{T}_d \boldsymbol{\tau} + \mathbf{B} \boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

with $\text{Cov}(\mathbf{y}) = \sigma^2 \mathbf{B} \mathbf{B}' + \mathbf{I}_n$ and with variable block sizes. He showed that balanced incomplete block designs which are universally optimal under the model without block effects and under the model with fixed block effects are not necessary universally optimal under the model with random block effects. In such a case competing designs have unequal block sizes. Observe that in model (5) the role of $\mathbf{B} \boldsymbol{\beta}$ is played by $\mathbf{L}_d \boldsymbol{\lambda}$, with an unequal number of replications instead of unequal block sizes.

4. D-optimality of Designs

In this section, we characterize D-optimal designs under the mixed interference model over the classes of complete block designs with $b = t - 2$ and $b = t$. The results are based on the paper by Filipiak et al. (2012).

Let $\tilde{\mathcal{P}}_t$ be the class of permutation matrices of order t with zeros on the diagonal (the class of derangement matrices) and let $\mathcal{B}_{r,b,k}$ be the class of binary designs. We define the following classes:

$$\tilde{\mathcal{B}}_{t,t-2,t} = \{d \in \mathcal{B}_{t,t-2,t} : \mathbf{S}_d = \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t - \mathbf{P}_d, \mathbf{P}_d \in \tilde{\mathcal{P}}_t\}$$

and

$$\hat{\mathcal{B}}_{t,t,t} = \{d \in \mathcal{B}_{t,t,t} : \mathbf{S}_d = \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t + \mathbf{P}_d, \mathbf{P}_d \in \tilde{\mathcal{P}}_t\}.$$

Observe that every derangement matrix \mathbf{P}_d is permutationally similar to the diagonal matrix $\text{diag}(\mathbf{H}_{t_1}, \dots, \mathbf{H}_{t_m})$, $\sum_{j=1}^m t_j = t$, $t_j \neq 1$, where m is the number of cycles in a permutation matrix and t_j is the length of the j th cycle. We should note that, if \mathbf{P}_d is permutationally similar to \mathbf{H}_t , then the designs from $\tilde{\mathcal{B}}_{t,t-2,t}$ and $\hat{\mathcal{B}}_{t,t,t}$ can be constructed from CNBDs with $b = t - 1$ by, respectively, removing and repeating one block. This follows from the form of the left-neighboring matrix of CNBD, i.e., if a design $d^\#$ is a CNBD with $b = t - 1$, then $\mathbf{S}_{d^\#} = \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t$; cf. Druilhet (1999).

Since designs from the class $\tilde{\mathcal{B}}_{t,t-2,t}$ and $\hat{\mathcal{B}}_{t,t,t}$ are binary and complete, the information matrix has the form (6).

4.1. D-optimality Over $\mathcal{R}_{t,t-2,t}$

Assume $d \in \tilde{\mathcal{B}}_{t,t-2,t}$ and $\mathbf{P}_d \in \tilde{\mathcal{P}}_t$. From (6)

$$\mathbf{C}_{d,\sigma} = \left(t - 2 - \frac{2\sigma_L^2}{1 + (t-2)\sigma_L^2} \right) \mathbf{I}_t - \frac{t-2 + t(t-4)\sigma_L^2}{t(1 + (t-2)\sigma_L^2)} \mathbf{1}_t \mathbf{1}'_t - \frac{\sigma_L^2}{1 + (t-2)\sigma_L^2} (\mathbf{P}_d + \mathbf{P}'_d).$$

Observe that the matrices $\mathbf{C}_{d,\sigma}$ and $\mathbf{C}_{d,\sigma} + \beta \mathbf{1}_t \mathbf{1}'_t$ have the same eigenvectors and that the eigenvalues corresponding to those eigenvectors are the same, except the vector $\mathbf{1}_t$, which is an eigenvector of both matrices corresponding to the eigenvalues 0 and βt , respectively. Thus the product of $t - 1$ eigenvalues of $\mathbf{C}_{d,\sigma}$ is equal to the determinant of $\mathbf{C}_{d,\sigma} + \beta \mathbf{1}_t \mathbf{1}'_t$ divided by βt , and it is enough to compare determinants of $\frac{1+(t-2)\sigma_L^2}{\sigma_L^2} \mathbf{C}_{d,\sigma} + \frac{t-2+t(t-4)\sigma_L^2}{t\sigma_L^2} \mathbf{1}_t \mathbf{1}'_t = \alpha \mathbf{I}_t - (\mathbf{P}_d + \mathbf{P}'_d)$ for different matrices \mathbf{P}_d , with $\alpha = t^2 - 4t + 2 + \frac{t-2}{\sigma_L^2}$.

For convenience, we denote the above matrix by $\tilde{\mathbf{C}}_{d,\sigma}$.

The following lemma will be useful in proving D-optimality results.

Lemma 1. (Filipiak et al., 2012) *If $\mathbf{P} \in \mathcal{P}_t$ is permutationally similar to \mathbf{H}_t , then $\det(\alpha \mathbf{I}_t - (\mathbf{P} + \mathbf{P}'))$, $\alpha > 2$, is maximal over \mathcal{P}_t .*

Now we state the following.

Theorem 2. *If there exists a design $d^* \in \tilde{\mathcal{B}}_{t,t-2,t}$, $t \geq 3$, such that the left-neighboring matrix \mathbf{S}_{d^*} is permutationally similar to $\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t - \mathbf{H}_t$, then d^* is D-optimal over $\mathcal{R}_{t,t-2,t}$, under the interference model \mathcal{M}_σ .*

Proof. Let d^* be a design such that \mathbf{S}_{d^*} is permutationally similar to $\mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t - \mathbf{H}_t$, $t \geq 3$. Due to Filipiak et al. (2012) we have

$$\det(\alpha \mathbf{I}_t - (\mathbf{H}_t + \mathbf{H}'_t)) = -2 + x^t + y^t \quad (9)$$

with

$$x = \frac{\alpha - \sqrt{\alpha^2 - 4}}{2}, \quad y = \frac{\alpha + \sqrt{\alpha^2 - 4}}{2}. \tag{10}$$

Observe that for $\alpha > 2$ the following inequalities hold:

$$0 < x < \frac{\alpha - (\alpha - 2)}{2} = 1, \quad \alpha - \frac{2}{\alpha} = \frac{\alpha + \alpha - \frac{4}{\alpha}}{2} < y < \frac{\alpha + \alpha}{2} = \alpha. \tag{11}$$

From (9), (11) and binomial evaluation

$$\begin{aligned} \det \tilde{\mathbf{C}}_{d^*, \sigma} &= \det (\alpha \mathbf{I}_t - (\mathbf{H}_t + \mathbf{H}'_t)) = \\ &= -2 + x^t + y^t > y^t - 2 > \left(\alpha - \frac{2}{\alpha}\right)^t - 2 > \alpha^t - 2t\alpha^{t-2} - 2. \end{aligned} \tag{12}$$

(a) Let $d \in \tilde{\mathcal{B}}_{t,t-2,t}$. Observe, that for $t \geq 4$ and $\sigma_L^2 \in (0, \infty]$ we have $\alpha > 2$ and the claim follows directly from Lemma 1. For $t = 3$ there is only one block in the design ($\mathbf{S}_d = \mathbf{P}_d$, $\mathbf{P}_d \in \tilde{\mathcal{P}}_t$) and from (6) it follows that $\mathbf{C}_{d,\sigma} = \frac{1}{1+\sigma_L^2} \mathbf{E}_3$ does not depend on the design.

(b) Let $d \in \mathcal{R}_{t,t-2,t} \setminus \tilde{\mathcal{B}}_{t,t-2,t}$. Due to (4) and (7) we may write

$$\tilde{\mathbf{C}}_{d,\sigma} \leq_L \left(\frac{t-2}{\sigma_L^2} + (t-2)^2 \right) \mathbf{I}_t - \mathbf{S}_d \mathbf{S}'_d + (t-4) \mathbf{1}_t \mathbf{1}'_t. \tag{13}$$

Recall that for every hermitian matrix the product of the eigenvalues of the matrix is majorized by the product of the diagonal entries of the matrix; cf. Marshall and Olkin (1979). Observe that the row and column sums of \mathbf{S}_d is $t-2$. Since for every $d \in \mathcal{R}_{t,t-2,t} \setminus \tilde{\mathcal{B}}_{t,t-2,t}$ at least one entry of \mathbf{S}_d is not smaller than 2, at least one diagonal entry of the matrix on the right-hand side of (13) is not greater than $\frac{t-2}{\sigma_L^2} + (t-2)^2 - t + (t-4) = \alpha - 2$, and the remaining diagonal entries are not greater than $\frac{t-2}{\sigma_L^2} + (t-2)^2 - (t-2) + (t-4) = \alpha$. Hence

$$\det \tilde{\mathbf{C}}_{d,\sigma} \leq \prod_{i=1}^t (\tilde{\mathbf{C}}_{d,\sigma})_{ii} \leq \alpha^{t-1} (\alpha - 2). \tag{14}$$

Comparing (12) and (14) we obtain

$$\alpha^{t-1} (\alpha - 2) - (\alpha^t - 2t\alpha^{t-2} - 2) = -2\alpha^{t-2} (t^2 - 6t + 2) + 2 \leq 0$$

for $t \geq 6$. If $t = 5$ we obtain the claim by comparing (14) with $(\alpha - \frac{2}{\alpha})^t - 2$.

Let $t = 4$. Then the design with the given structure of left-neighboring matrix cannot exist. The only design from the class $\tilde{\mathcal{B}}_{4,2,4}$ is a design with the left-neighboring matrix permutationally similar to $\mathbf{1}_4 \mathbf{1}'_4 - \mathbf{I}_4 - \mathbf{H}_4^2$. For example, such a design has the form: $d_1 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 3 & 2 \end{pmatrix}$. The remaining designs can be constructed by relabeling treatments in this design. D-optimality of d_1 is proved by direct comparison of d_1 with all equireplicated designs.

For $t = 3$ all designs from $\mathcal{R}_{3,1,3} \setminus \tilde{\mathcal{B}}_{3,1,3}$ are disconnected. □

We should note that under the fixed interference model the designs given in Theorem 2 are D-optimal over the class $\mathcal{D}_{t,t-2,t}$; cf. Filipiak et al. (2012).

4.2. D-optimality Over $\overline{\mathcal{R}}_{t,t,t}$

Assume $d \in \widehat{\mathcal{B}}_{t,t,t}$ and $\mathbf{P}_d \in \widetilde{\mathcal{P}}_t$. From (6)

$$\mathbf{C}_{d,\sigma} = \left(t - \frac{2\sigma_L^2}{1+t\sigma_L^2} \right) \mathbf{I}_t - \mathbf{1}_t \mathbf{1}'_t + \frac{\sigma_L^2}{1+t\sigma_L^2} (\mathbf{P}_d + \mathbf{P}'_d).$$

Similarly as in the previous sections, to characterize a D-optimal design it is enough to compare the determinants of $\frac{1+t\sigma^2}{\sigma^2} (\mathbf{C}_{d,\sigma} + \mathbf{1}_t \mathbf{1}'_t) = \alpha \mathbf{I}_t + \mathbf{P}_d + \mathbf{P}'_d$, $\alpha = t^2 - 2 + \frac{t}{\sigma^2}$, for different matrices \mathbf{P}_d . For convenience, we denote the above matrix by $\widehat{\mathbf{C}}_{d,\sigma}$.

The following lemma will be useful in proving D-optimality results.

Lemma 2. [Filipiak et al., 2012] If $\mathbf{P} \in \widetilde{\mathcal{P}}_t$ is permutationally similar to

- (i) $\mathbf{I}_m \otimes \mathbf{H}_3$, for $t = 3m$, $m \in \mathbb{N} \setminus \{1\}$;
 - (ii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_4)$, for $t = 3m + 4$, $m \in \mathbb{N}$;
 - (iii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_5)$, for $t = 3m + 5$, $m \in \mathbb{N}$,
- then $\det(\alpha \mathbf{I}_t + \mathbf{P} + \mathbf{P}')$, $\alpha \geq 2.5$, is maximal over $\widetilde{\mathcal{P}}_t$. Moreover, if $2 \leq t \leq 5$ then the determinant of $\alpha \mathbf{I}_t + \mathbf{H}_t + \mathbf{H}'_t$ is maximal over $\widetilde{\mathcal{P}}_t$ for $\alpha > 2$.

Now we state the following.

Theorem 3. If there exists a design $d^* \in \widehat{\mathcal{B}}_{t,t,t}$, $t \geq 3$, such that \mathbf{S}_{d^*} is permutationally similar to

- (i) $\mathbf{I}_m \otimes \mathbf{H}_3 + \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t$, for $t = 3m$, $m \in \mathbb{N}$;
 - (ii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_4) + \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t$, for $t = 3m + 4$, $m \in \mathbb{N} \cup \{0\}$;
 - (iii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_5) + \mathbf{1}_t \mathbf{1}'_t - \mathbf{I}_t$, for $t = 3m + 5$, $m \in \mathbb{N} \cup \{0\}$,
- then d^* is D-optimal over $\overline{\mathcal{R}}_{t,t,t}$ under the interference model \mathcal{M}_σ .

Proof. Let d^* be a design such that \mathbf{S}_{d^*} is permutationally similar to the respective matrix from the theorem. Due to Filipiak et al. (2012) we obtain

$$\det(\alpha \mathbf{I}_t + \mathbf{H}_t + \mathbf{H}'_t) = \begin{cases} -2 + x^t + y^t, & \text{for even } t, \\ 2 + x^t + y^t, & \text{for odd } t, \end{cases} \quad (15)$$

with x and y defined in (10). Observe that for $\alpha \geq 2.13$ the following inequalities are valid:

$$0 < x \leq \frac{\alpha - (\alpha - 1)}{2} = \frac{1}{2}, \quad \alpha - \frac{3}{2\alpha} = \frac{\alpha + \alpha - 1}{2} \leq y < \frac{\alpha + \alpha}{2} = \alpha. \quad (16)$$

From (15) we have

$$\det \widehat{\mathbf{C}}_{d^*,\sigma} = \begin{cases} (2 + x^3 + y^3)^m, & \text{for } t = 3m, m \in \mathbb{N}, \\ (2 + x^3 + y^3)^m (-2 + x^4 + y^4), & \text{for } t = 3m + 4, m \in \mathbb{N} \cup \{0\}, \\ (2 + x^3 + y^3)^m (2 + x^5 + y^5), & \text{for } t = 3m + 5, m \in \mathbb{N} \cup \{0\}. \end{cases}$$

Using (16) we may write

$$\det \widehat{\mathbf{C}}_{d^*,\sigma} > \begin{cases} y^t - 2y^{t-4}, & \text{for } t = 3m + 4, m \in \mathbb{N} \cup \{0\}, \\ y^t, & \text{for remaining } t. \end{cases}$$

It is easy to see that $\det \widehat{\mathbf{C}}_{d^*,\sigma} > y^t - 2y^{t-4}$. Observe that since $\alpha > 7$, $y > \alpha - \frac{3}{2\alpha}$. Thus, using binomial evaluation,

$$\det \widehat{\mathbf{C}}_{d^*,\sigma} > \left(\alpha - \frac{3}{2\alpha}\right)^{t-4} (\alpha^4 - 6\alpha^2 + \frac{23}{2} + \frac{81}{16\alpha^4} - \frac{27}{2\alpha^2}) > (\alpha^{t-4} - \frac{3(t-4)}{2}\alpha^{t-6}) (\alpha^4 - 6\alpha^2).$$

(a) Let $d \in \widehat{\mathcal{B}}_{t,t,t}$. Observe that for every $t \geq 3$ the parameter $\alpha > 2.5$ and the claim follows directly from Lemma 2.

(b) Let $d \in \overline{\mathcal{R}}_{t,t,t} \setminus \widehat{\mathcal{B}}_{t,t,t}$. Due to (4) and (7) we may write

$$\widehat{\mathbf{C}}_{d,v} \leq_L \left(\frac{t}{\sigma_L^2} + t^2\right) \mathbf{I}_t - \mathbf{S}_d \mathbf{S}'_d + t \mathbf{1}_t \mathbf{1}'_t.$$

Observe that at least t off-diagonal entries of \mathbf{S}_d are not smaller than 2, or at least one entry of \mathbf{S}_d is greater than 2 and in both cases at least one off-diagonal entry of \mathbf{S}_d is zero. Thus at least one diagonal entry of $\widehat{\mathbf{C}}_{d,\sigma}$ is not greater than $t^2 + \frac{t}{\sigma^2} - (4 + 4 + t - 4) + t = \alpha - 2$, and the remaining diagonal entries are not greater than α . We obtain

$$\det(\widehat{\mathbf{C}}_{d,\sigma}) \leq \prod_{i=1}^t (\widehat{\mathbf{C}}_{d,\sigma})_{ii} \leq \alpha^{t-1} (\alpha - 2).$$

It is enough to show that

$$\alpha^t - 2\alpha^{t-1} \leq \left(\alpha^{t-4} - \frac{3(t-4)}{2}\alpha^{t-6}\right) (\alpha^4 - 6\alpha^2).$$

We obtain

$$\begin{aligned} &\alpha^t - 2\alpha^{t-1} - \left(\alpha^{t-4} - \frac{3(t-4)}{2}\alpha^{t-6}\right) (\alpha^4 - 6\alpha^2) = \\ &= -\alpha^{t-4} \left(2\alpha^3 - \frac{3}{2}t\alpha^2 + 9(t-4)\right) = \\ &= -\alpha^{t-4} \left(2t^6 - 3t^5 - 12t^4 + 12t^3 + 24t^2 - 3t - 52 + \right. \\ &\quad \left. + \frac{t(2t^2 + 3t\sigma^2(2t^2 - t - 4) + 6\sigma^4(t^4 - t^3 - 4t^2 + 2t + 4))}{\sigma^6}\right). \end{aligned} \tag{17}$$

Observe that both $2t^6 - 3t^5 - 12t^4 + 12t^3 + 24t^2 - 3t - 52$ as well as $2t^2 + 3t\sigma^2(2t^2 - t - 4) + 6\sigma^4(t^4 - t^3 - 4t^2 + 2t + 4)$ are positive for every $t \geq 3$ and the expression in (17) is negative. \square

We should note that under the fixed interference model the designs given in Theorem 3 are D-optimal over the class $\mathcal{D}_{t,t-2,t}$; cf. Filipiak et al. (2012).

4.3. Remarks

Since the following relation holds between the information matrices $\mathbf{C}_{d,u}$, $u \in \{0, \sigma, \infty\}$:

$$\mathbf{C}_{d,\infty} \leq_L \mathbf{C}_{d,\sigma} \leq_L \mathbf{C}_{d,0}$$

(cf. Markiewicz, 1997), all the results for model \mathcal{M}_σ hold also for model \mathcal{M}_∞ . Moreover, since the designs which satisfy the conditions of Theorem 4.1 and Theorem 4.2 are binary and complete, they are balanced with respect to the blocks. Such designs are universally optimal over $\mathcal{D}_{t,b,t}$ under the model \mathcal{M}_0 ; see, e.g., Shah and Sinha (1989).

From Filipiak et al. (2012) it follows that D-optimal designs under the fixed and mixed interference models have the same structure of left-neighboring matrices. Thus all the construction methods may be applied.

Recall that a D-optimal design from $\mathcal{R}_{t,t-2,t}$ can be constructed from a CNBD by removing one arbitrary block. A catalogue of CNBDs with $t = k$, $b = t - 1$ is given in Azaïs et al. (1993). Observe, however, that for $t = 6$ a CNBD with $b = t - 1$ and $t = k$ cannot exist. Moreover, numerical calculations show that a design with $\mathbf{S}_d = \mathbf{1}_6 \mathbf{1}'_6 - \mathbf{I}_6 - \mathbf{H}_6$ does not exist either. In the class $\tilde{\mathcal{B}}_{6,4,6}$ there exist only designs with left-neighboring matrix permutationally similar to $\mathbf{1}_6 \mathbf{1}'_6 - \mathbf{I}_6 - \text{diag}(\mathbf{H}_4 : \mathbf{H}_2)$ (say \mathbf{S}_{d_1}) or $\mathbf{1}_6 \mathbf{1}'_6 - \mathbf{I}_6 - \mathbf{I}_3 \otimes \mathbf{H}_2$ (say \mathbf{S}_{d_2}). For such designs we have

$$\begin{aligned} \det \tilde{\mathbf{C}}_{d_1, \sigma} - \det \tilde{\mathbf{C}}_{d_2, \sigma} &= \\ &= \frac{1024(1 + 4\sigma_L^2)^2(21\sigma_L^4 + 13\sigma_L^4 + 2)^2}{\sigma_L^{12}} - \frac{4096(1 + 4\sigma_L^2)^3(1 + 3\sigma_L^2)^3}{\sigma_L^{12}} = \\ &= \frac{1024(1 + 4\sigma_L^2)^2(1 + 3\sigma_L^2)^2}{\sigma_L^8} > 0 \end{aligned}$$

for every $\sigma_L^2 \in (0, \infty]$. Moreover, for a design $d \in \mathcal{R}_{6,4,6}$, from (14)

$$\det \tilde{\mathbf{C}}_{d, \sigma} \leq \alpha^5(\alpha - 2) = \frac{128(1 + 3\sigma_L^2)(2 + 7\sigma_L^2)^5}{\sigma_L^{12}}$$

and

$$\det \tilde{\mathbf{C}}_{d_1, \sigma} - \det \tilde{\mathbf{C}}_{d, \sigma} \geq \frac{128(2 + 7\sigma_L^2)^2(123\sigma_L^6 + 119\sigma_L^4 + 38\sigma_L^2 + 4)}{\sigma_L^{10}} > 0$$

for every $\sigma_L^2 \in (0, \infty]$. Thus the design d_1 is D-optimal over $\mathcal{R}_{6,4,6}$.

Example 3. The following design is D-optimal over $\mathcal{R}_{6,4,6}$:

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

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