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D–OPTIMAL BIASED CHEMICAL BALANCE WEIGHING DESIGNS

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Dedicated to the memory of Professor Wiktor Oktaba

Summary

In this paper, we consider the D–optimal chemical balance weighing designs for estimation of individual unknown weights of objects. We assume that the error terms create a first–order autoregressive process. Then the covariance matrix of errors has known form, which does not have to be identity matrix and depends on known parameter ρ. In the literature, some results about the D–optimal designs, when there are three objects are known. We present the biased chemical balance weighing design given by its design matrix and we prove that it is D–optimal biased design in some class of designs, if the number of objects is three and $\rho \geq 0$. For such ρ, we show also the theorem giving the necessary and sufficient condition under which the biased design for three objects is D–optimal. Finally, we describe some relations between D–optimal designs and D–optimal biased designs for three objects and $\rho \geq 0$.

Key words and phrases: chemical balance weighing design, D–optimality, first–order autoregressive process

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1. Introduction

In a weighing design problem, the goal is to determine the weights of p objects in a given number of weighings. In many papers, the balance weighing designs are discussed and some examples of applying these designs in the agricultural experiments are presented (see for example Banerjee (1975), Katulska (1984), Ceranka and Katulska (1987)).

The paper deals with a chemical balance. There are two pans (left and right) and any object can be placed on one of them. A reading represents the total weight of the objects on the pans. We would like to choose a chemical balance weighing design that is optimal with respect to some criterion. In the literature, there are several optimality criteria of measure the quality of weighing designs. We are interested in the D–optimality criterion. It is defined below.

Suppose that $n \equiv 0 \pmod 4$. There are p objects of the true unknown weights $w_1, w_2, \ldots, w_p$, respectively. We estimate them employing n measuring operations using a chemical balance. Assume that $y_1, y_2, \ldots, y_n$ denote the observations in these n operations, respectively. Let the observations follow the linear model $\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\varepsilon}$, where $\mathbf{y} = [y_1, y_2, \ldots, y_n]'$ is an $n \times 1$ vector of observations, $\mathbf{w} = [w_1, w_2, \ldots, w_p]'$ is the vector of unknown weights of objects, the $n \times p$ matrix $\mathbf{X} = [x_{ij}]$ is called the design matrix and $x_{ij} = -1$ $(x_{ij} = 1)$ if the jth object is placed on the left (right) pan during the ith weighing operation, the vector $\boldsymbol{\varepsilon} = [\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n]'$ is the vector of error components such that $E(\boldsymbol{\varepsilon}) = [0, 0, \ldots, 0]'$ is an $n \times 1$ vector of zeros and $Var(\boldsymbol{\varepsilon}) = \frac{1}{1-\rho^2}\mathbf{S}$, where $\mathbf{S} = (\rho^{|r-d|})_{r,d=1}^{n}$ and $-1 < \rho < 1$. We identify the design with its design matrix $\mathbf{X}$. If the first column of a design matrix $\mathbf{X}$ contains only ones, then such design is called a biased chemical balance weighing design for $p-1$ objects.

Vector of unknown weights $\mathbf{w}$ is estimated using the normal equations of the form $\mathbf{X}'\mathbf{S}^{-1}\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{S}^{-1}\mathbf{y}$. The chemical balance weighing design is singular (nonsingular) if the information matrix $\mathbf{X}'\mathbf{S}^{-1}\mathbf{X}$ is singular (nonsingular). If the design is nonsingular, then the generalized least–squares estimator of the vector $\mathbf{w}$ is equal to $\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{S}^{-1}\mathbf{y}$. The covariance matrix of $\hat{\mathbf{w}}$ is given by the formula $Var(\hat{\mathbf{w}}) = \frac{1}{1-\rho^2}(\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})^{-1}$. The inverse of the matrix $\mathbf{S}$ is equal to $\mathbf{S}^{-1} = \frac{1}{1-\rho^2}\mathbf{A}$, where

$$\mathbf{A} = \begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 & 0 \\ 0 & -\rho & 1+\rho^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1+\rho^2 & -\rho \\ 0 & 0 & 0 & \cdots & -\rho & 1 \end{bmatrix}. \tag{1.1}$$

The matrix $\mathbf{A}$ is positive definite for $\rho \in (-1, 1)$.

We consider the D–optimal chemical balance weighing designs, which maximize the determinant of the information matrix. We say that the design $\tilde{\mathbf{X}}$ is D–optimal in the class of the designs C, where C is a subset of the set $M_{n\times p}(\pm 1)$ of all matrices with n rows, p columns and elements 1 or -1, if $\det(\tilde{\mathbf{X}}'\mathbf{S}^{-1}\tilde{\mathbf{X}}) = \max\{\det(\mathbf{X}'\mathbf{S}^{-1}\mathbf{X}) : \mathbf{X} \in C\}$. It is easy to see that the design $\tilde{\mathbf{X}}$ is D–optimal in the class of designs $C \subseteq M_{n\times p}(\pm 1)$, if $\det(\tilde{\mathbf{X}}'\mathbf{A}\tilde{\mathbf{X}}) = \max\{\det(\mathbf{X}'\mathbf{A}\mathbf{X}) : \mathbf{X} \in C\}$, where $\mathbf{A}$ is in form (1.1). If the error components have a normal distribution, then D–optimal design minimizes the expected volume of the usual confidence ellipsoid for $\mathbf{w}$.

When the matrix $\mathbf{S}$ is the identity matrix $(\rho = 0)$, D–optimal designs are considered in many papers (see for example Cheng 1980, Galil and Kiefer 1980, or Jacroux et. al. 1983). For $\rho \neq 0$, Li and Yang (2005) and Yeh and Lo Huang (2005) proved some theorems about D–optimal biased designs, if $p = 3$. For $-1 < \rho \le 0$ and $p = 3$, Katulska and Smaga (2010) presented some construction of D–optimal design in the class of designs such that each column of the design matrix contains at least one 1 and one -1. Some results about D–optimality problem for some $\rho \in [0, 1)$ in the class of designs $M_{n\times 3}(\pm 1)$ are given in Katulska and Smaga (to appear).

In this paper, we prove that the design with the design matrix

$$\hat{\mathbf{X}}=\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & 1_2 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1_1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1_3 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}, \textit{if } n/4=2k-1, \quad \hat{\mathbf{X}}=\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1_2 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1_1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1_3 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}, \textit{if } n/4=2k, \quad (1.2)$$

where $k=1,2,\ldots$ and elements with indices $1, 2$ and 3 are in positions $(n/2,3),(n/4,4),(3n/4,4),$ respectively, is D–optimal in certain class of biased designs, if $p=4$ and $\rho \geq 0$. The necessary and sufficient condition under which the design is D–optimal in that class is also given. At the end, we present some relations between the D–optimal designs for three objects $(p=3)$ from Katulska and Smaga (to appear) and the D–optimal biased designs for three objects $(p=4)$ given in this paper.

2. Preliminaries

This section contains some definitions, lemmas and theorem, which are used inSection 3. For any vector $\mathbf{x} = [x_1, x_2, \ldots, x_n]' \in M_{n\times 1}(\pm 1)$, we define the numbers

$cons(\mathbf{x}) = \#\{i : x_i = x_{i+1}, 1 \le i \le n-1\}$,

$fcons(\mathbf{x}) = \min\{i : x_i = x_{i+1}, 1 \le i \le n-1\}$,

$scons(\mathbf{x}) = \min\{i : i > fcons(\mathbf{x}), x_i = x_{i+1}, 1 \le i \le n-1\}$.

Lemma 2.1. For $\mathbf{X} \in M_{n\times p}(\pm 1)$ and $n \times n$ real matrix $\mathbf{G}$, the determinant of the matrix $\mathbf{X}'\mathbf{G}\mathbf{X}$ does not change if we interchange two columns of the matrix $\mathbf{X}$ or we multiply any column of this matrix by -1.

Theorem 2.1. (Hadamard's inequality) If $\mathbf{P} = [p_{ij}]$ is an $n \times n$ positive semi–definite matrix, then

$$\det(\mathbf{P}) \le \prod_{i=1}^{n} p_{ii}.$$

Lemma 2.2. Let $n \equiv 0 \pmod 4$ and $\lambda = 0, 1, 2, \ldots, n-1$.
If $\Delta = (n-2)(1+\rho)^2 + 2(1+\rho)$, $\rho \ne 0$ and $\mathbf{x} \in M_{n\times 1}(\pm 1)$, then $cons(\mathbf{x}) = \lambda$ if and only if $\mathbf{x}'\mathbf{A}\mathbf{x} = \Delta - 4\lambda\rho$.

Lemma 2.3. Assume that
$\mathbf{x} = [x_1, x_2, \ldots, x_n]'$, $\mathbf{y} = [y_1, y_2, \ldots, y_n]' \in M_{n\times 1}(\pm 1)$, $n \equiv 0 \pmod 4$.

(a) If $cons(\mathbf{x}) = 0$, $cons(\mathbf{y}) = 2$, $a = fcons(\mathbf{y})$, $b = scons(\mathbf{y})$, then

$$\mathbf{x}'\mathbf{A}\mathbf{y} = \begin{cases} (n+2a-2b-2)(1+\rho)^2 + 2(1+\rho) & if\ x_1 = y_1 \\ -((n+2a-2b-2)(1+\rho)^2 + 2(1+\rho)) & if\ x_1 \ne y_1 \end{cases}.$$

(b) If $cons(\mathbf{x}) = 0$, $cons(\mathbf{y}) = 1$, $a = fcons(\mathbf{y})$, then

$$\mathbf{x}'\mathbf{A}\mathbf{y} = \begin{cases} (2a-n)(1+\rho)^2 & if\ x_1 = y_1 \\ -(2a-n)(1+\rho)^2 & if\ x_1 \ne y_1 \end{cases}.$$

(c) If $\mathbf{1} = [1, 1, \ldots, 1]'$, $cons(\mathbf{x}) = 2$, $a = fcons(\mathbf{x})$, $b = scons(\mathbf{x})$, then

$$\mathbf{1}'\mathbf{A}\mathbf{x} = \begin{cases} 2(1-\rho)^2 & if\ (a\ even, b\ odd, x_1 = -1)\ or\ (a\ odd, b\ even, x_1 = 1) \\ -2(1-\rho)^2 & if\ (a\ even, b\ odd, x_1 = 1)\ or\ (a\ odd, b\ even, x_1 = -1) \\ 0 & if\ (a\ even, b\ even)\ or\ (a\ odd, b\ odd) \end{cases}.$$

(d) If $\mathbf{1} = [1, 1, \ldots, 1]'$, $cons(\mathbf{x}) = 1$, $a = fcons(\mathbf{x})$, then

$$\mathbf{1}'\mathbf{A}\mathbf{x} = \begin{cases} 2(1-\rho) & if\ a\ odd, x_1 = 1 \\ -2(1-\rho) & if\ a\ odd, x_1 = -1 \\ 2\rho(1-\rho) & if\ a\ even, x_1 = 1 \\ -2\rho(1-\rho) & if\ a\ even, x_1 = -1 \end{cases}.$$

3. Main results

In this section, we formulate new theorems concerning D–optimal biased chemical balance weighing designs. In the first theorem, we prove that the design $\hat{\mathbf{X}}$ given by (1.2) is D–optimal in some large subclass of the class of designs $\mathbf{X} = [\mathbf{1} \mid \mathbf{x} \mid \mathbf{y} \mid \mathbf{z}] \in M_{n\times 4}(\pm 1)$ for all $\rho \in [0, 1)$. For the design matrix $\hat{\mathbf{X}}$ of the form (1.2), we have

$$\det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) = \det\begin{bmatrix} \delta & 0 & 2\rho(1-\rho) & 0 \\ 0 & \Delta & 0 & -2\rho(1+\rho) \\ 2\rho(1-\rho) & 0 & \Delta - 4\rho & 0 \\ 0 & -2\rho(1+\rho) & 0 & \Delta - 8\rho \end{bmatrix}$$

$$= \delta(\Delta - 4\rho)[\Delta(\Delta - 8\rho) - 4\rho^2(1+\rho)^2]$$

$$+16\rho^4(1-\rho)^2(1+\rho)^2 - 4\rho^2(1-\rho)^2\Delta(\Delta - 8\rho),$$

where $\delta = \mathbf{1}'\mathbf{A}\mathbf{1} = (n-2)(1-\rho)^2 + 2(1-\rho)$, $\Delta = (n-2)(1+\rho)^2 + 2(1+\rho)$.

Theorem 3.1. If $n \equiv 0 \pmod 4$ and $\rho \in [0, 1)$, then the design with the design matrix $\hat{\mathbf{X}}$ given by (1.2) is D–optimal in the class of designs with the design matrix $\mathbf{X} = [\mathbf{1} \mid \mathbf{x} \mid \mathbf{y} \mid \mathbf{z}] \in M_{n\times 4}(\pm 1)$ such that $rank(\mathbf{X}) = 4$ and

$$cons(\mathbf{x}) \geq 0, cons(\mathbf{y}) \geq 1, cons(\mathbf{z}) \geq 2 \text{ or } cons(\mathbf{x}) = 1, cons(\mathbf{y}) = 1, cons(\mathbf{z}) = 1.$$

Proof. (Sketch) If $n = 4$, then

$$\det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) = \det(\hat{\mathbf{X}}')\det(\mathbf{A})\det(\hat{\mathbf{X}}) = \det(\hat{\mathbf{X}}'\hat{\mathbf{X}})\det(\mathbf{A}) = n^4 \det(\mathbf{A})$$

so from Hadamard (1893) the design matrix $\hat{\mathbf{X}}$ is D–optimal. When $\rho = 0$, then $\hat{\mathbf{X}}$ is also D–optimal, since $\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}} = \hat{\mathbf{X}}'\hat{\mathbf{X}} = n\mathbf{I}_4$.
Let us assume that $n \geq 8$ and $\rho \in (0, 1)$. It is clear that the matrix $\mathbf{X}'\mathbf{A}\mathbf{X}$ is positive definite. By Lemma 2.1, we can assume $x_1 = y_1 = z_1 = 1$ and consider only the class of designs with design matrices in the sum $C_1 \cup C_2 \cup C_3 \cup C_4 \cup C_5$, where

$$C_1 = \{[\mathbf{1} \mid \boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 4}(\pm 1) : cons(\boldsymbol{\alpha}) \geq 1, cons(\boldsymbol{\beta}) \geq 1, cons(\boldsymbol{\gamma}) \geq 2\},$$

$$C_2 = \{[\mathbf{1} \mid \boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 4}(\pm 1) : cons(\boldsymbol{\alpha}) = 0, cons(\boldsymbol{\beta}) \geq 2, cons(\boldsymbol{\gamma}) \geq 2\},$$

$$C_3 = \{[\mathbf{1} \mid \boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 4}(\pm 1) : cons(\boldsymbol{\alpha}) = 0, cons(\boldsymbol{\beta}) = 1, cons(\boldsymbol{\gamma}) \geq 3\},$$

$$C_4 = \{[\mathbf{1} \mid \boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 4}(\pm 1) : cons(\boldsymbol{\alpha}) = 0, cons(\boldsymbol{\beta}) = 1, cons(\boldsymbol{\gamma}) = 2\},$$

$$C_5 = \{[\mathbf{1} \mid \boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 4}(\pm 1) : cons(\boldsymbol{\alpha}) = 1, cons(\boldsymbol{\beta}) = 1, cons(\boldsymbol{\gamma}) = 1\}.$$

We divide the proof into five cases and in *i*–th case, $i = 1, 2, \ldots, 5$, we show that $\det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) \geq \det(\mathbf{X}'\mathbf{A}\mathbf{X})$ for all $\mathbf{X} \in C_i$. For example, we present the proof in Case 1.

Case 1. Let $\mathbf{X} = [\mathbf{1} \mid \mathbf{x} \mid \mathbf{y} \mid \mathbf{z}] \in C_1$. By Hadamard's inequality, we obtain

$$\det(\mathbf{X}'\mathbf{AX}) = \det\begin{bmatrix} \mathbf{1}'\mathbf{A1} & \mathbf{1}'\mathbf{Ax} & \mathbf{1}'\mathbf{Ay} & \mathbf{1}'\mathbf{Az} \\ \mathbf{x}'\mathbf{A1} & \mathbf{x}'\mathbf{Ax} & \mathbf{x}'\mathbf{Ay} & \mathbf{x}'\mathbf{Az} \\ \mathbf{y}'\mathbf{A1} & \mathbf{y}'\mathbf{Ax} & \mathbf{y}'\mathbf{Ay} & \mathbf{y}'\mathbf{Az} \\ \mathbf{z}'\mathbf{A1} & \mathbf{z}'\mathbf{Ax} & \mathbf{z}'\mathbf{Ay} & \mathbf{z}'\mathbf{Az} \end{bmatrix} \le (\mathbf{1}'\mathbf{A1})(\mathbf{x}'\mathbf{Ax})(\mathbf{y}'\mathbf{Ay})(\mathbf{z}'\mathbf{Az}).$$

From Lemma 2.2, the inequalities

$$\mathbf{x}'\mathbf{Ax} \le \Delta - 4\rho,\ \mathbf{y}'\mathbf{Ay} \le \Delta - 4\rho,\ \mathbf{z}'\mathbf{Az} \le \Delta - 8\rho$$

hold. Hence $\det(\mathbf{X}'\mathbf{AX}) \le \delta(\Delta - 4\rho)^2(\Delta - 8\rho)$ and

$$\begin{aligned} \det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) - \det(\mathbf{X}'\mathbf{AX}) &\ge \det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) - \delta(\Delta - 4\rho)^2(\Delta - 8\rho) \\ &\ge \delta(\Delta - 4\rho)[4\rho(\Delta - 8\rho) - 4\rho^2(1+\rho)^2] \\ &\quad - 4\rho^2(1-\rho)^2\Delta(\Delta - 4\rho) + 16\rho^3(1-\rho)^2\Delta \\ &\ge 4\rho(\Delta - 4\rho)[\delta(\Delta - 8\rho) - \delta\rho(1+\rho)^2 - \rho(1-\rho)^2\Delta] \\ &= 4\rho(1-\rho)(\Delta - 4\rho)[(n-2)(1-\rho)(1+\rho)^2\{n - 2(1-\rho)\} + 4(1-\rho^2) \\ &\quad + 2\{4(n-2)\rho^2 + (-2(n+2))\rho + 2(n-2)\}] > 0. \end{aligned}$$

The proof is finished. ■

In the below theorem, we consider the whole class of designs $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1)$ and we show that the design $\hat{\mathbf{X}}$ of the form (1.2) is still D–optimal in this class if $\rho \in [0, 1/(n-2)]$. The proof of that theorem is based on the similar idea as the proof of Theorem 3.1.

Theorem 3.2. Let $\rho \in [0, 1/(n-2)]$ and $n \equiv 0 \pmod 4$. The D–optimal design in the class of designs with the design matrix $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1)$, $rank(\mathbf{X}) = 4$ is the design $\hat{\mathbf{X}}$ given by (1.2).

Theorem below was proved in Katulska and Smaga (to appear).

Theorem 3.3.
If $n \equiv 0 \pmod 4$, $\rho \in [0, 1/(n-2))$, $\mathbf{X}^* = [\mathbf{x}^* \,|\, \mathbf{y}^* \,|\, \mathbf{z}^*] \in M_{n\times 3}(\pm 1)$ and $rank(\mathbf{X}^*) = 3$, then the design $\mathbf{X}^*$ is D–optimal in the class of designs $\mathbf{X} \in M_{n\times 3}(\pm 1)$, $rank(\mathbf{X}) = 3$ if and only if

$$\mathbf{X}^{*\prime}\mathbf{A}\mathbf{X}^* = \begin{bmatrix} \Delta & 0 & \pm 2\rho(1+\rho) \\ 0 & \Delta - 4\rho & 0 \\ \pm 2\rho(1+\rho) & 0 & \Delta - 8\rho \end{bmatrix}$$

exact to permuting columns of the matrix $\mathbf{X}^*$.

For D–optimal biased chemical balance weighing designs for three objects $(p = 4)$, we can prove similar result and we formulate it in Theorem 3.4.

Theorem 3.4. Let $n \equiv 0 \pmod 4$,

$$\rho \in [0, 1/(n-2)],\ \tilde{\mathbf{X}} = [\mathbf{1} \,|\, \mathbf{X}^*] = [\mathbf{1} \,|\, \mathbf{x}^* \,|\, \mathbf{y}^* \,|\, \mathbf{z}^*] \in M_{n\times 4}(\pm 1)$$

and $rank(\tilde{\mathbf{X}}) = 4$. The design $\tilde{\mathbf{X}}$ is D–optimal in the class of designs $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1)$, $rank(\mathbf{X}) = 4$ if and only if

$$\tilde{\mathbf{X}}'\mathbf{A}\tilde{\mathbf{X}} = \begin{bmatrix} \delta & 0 & \pm 2\rho(1-\rho) & 0 \\ 0 & \Delta & 0 & \pm 2\rho(1+\rho) \\ \pm 2\rho(1-\rho) & 0 & \Delta - 4\rho & 0 \\ 0 & \pm 2\rho(1+\rho) & 0 & \Delta - 8\rho \end{bmatrix} \tag{3.1}$$

exact to permuting columns of the matrix $\tilde{\mathbf{X}}$ and the sign of element in (1,3)–position is independent on the sign of element in (2,4)–position.

The proof of the above theorem is based on the proofs of Theorems 3.1 and 3.2. Now, we present some relations between D–optimal designs described in Theorem 3.3 and Theorem 3.4.

Theorem 3.5. Assume that $n \equiv 0 \pmod 4$, $\rho \in (0, 1/(n-2))$ and $\mathbf{X}^* = [\mathbf{x}^* \,|\, \mathbf{y}^* \,|\, \mathbf{z}^*] \in M_{n\times 3}(\pm 1)$ is such that $rank([\mathbf{1} \,|\, \mathbf{X}^*]) = 4$. If the design $\mathbf{X}^*$ is D–optimal in the class of designs $M_{n\times 3}(\pm 1)$, then the design

$\tilde{\mathbf{X}} = [\mathbf{1} \,|\, \mathbf{X}^*]$ is D–optimal in the class of designs $[\mathbf{1} \,|\, \mathbf{X}] \in M_{n\times 4}(\pm 1),\ rank([\mathbf{1} \,|\, \mathbf{X}]) = 4.$

Proof. Let $\mathbf{X}^* = [\mathbf{x}^* \,|\, \mathbf{y}^* \,|\, \mathbf{z}^*]$ be D–optimal design in the class of designs $M_{n\times 3}(\pm 1)$ and $\tilde{\mathbf{X}} = [\mathbf{1} \,|\, \mathbf{X}^*]$. From Theorem 3.3 we obtain

$$\tilde{\mathbf{X}}'\mathbf{A}\tilde{\mathbf{X}} = \begin{bmatrix} \mathbf{1}'\mathbf{A}\mathbf{1} & \mathbf{1}'\mathbf{A}\mathbf{X}^* \\ \mathbf{X}^{*}{}'\mathbf{A}\mathbf{1} & \mathbf{X}^{*}{}'\mathbf{A}\mathbf{X}^* \end{bmatrix} = \begin{bmatrix} \delta & \mathbf{1}'\mathbf{A}\mathbf{x}^* & \mathbf{1}'\mathbf{A}\mathbf{y}^* & \mathbf{1}'\mathbf{A}\mathbf{z}^* \\ \mathbf{x}^{*}{}'\mathbf{A}\mathbf{1} & \Delta & 0 & \pm 2\rho(1+\rho) \\ \mathbf{y}^{*}{}'\mathbf{A}\mathbf{1} & 0 & \Delta - 4\rho & 0 \\ \mathbf{z}^{*}{}'\mathbf{A}\mathbf{1} & \pm 2\rho(1+\rho) & 0 & \Delta - 8\rho \end{bmatrix}.$$

From Lemma 2.2 follows that

$$\mathbf{x}^{*}{}'\mathbf{A}\mathbf{x}^* = \Delta \Leftrightarrow cons(\mathbf{x}^*) = 0,\ \mathbf{y}^{*}{}'\mathbf{A}\mathbf{y}^* = \Delta - 4\rho \Leftrightarrow cons(\mathbf{y}^*) = 1$$

and $\mathbf{z}^{*}{}'\mathbf{A}\mathbf{z}^* = \Delta - 8\rho \Leftrightarrow cons(\mathbf{z}^*) = 2.$

Condition $cons(\mathbf{x}^*) = 0$ implies $\mathbf{1}'\mathbf{A}\mathbf{x}^* = 0.$ Moreover, from Lemma 2.3 (b), we have that $\mathbf{x}^{*}{}'\mathbf{A}\mathbf{y}^* = \pm(2a - n)(1+\rho)^2 = 0,$ where $a = fcons(\mathbf{y}^*).$ So $a = n/2$ and by (d) in Lemma 2.3 it follows that $\mathbf{1}'\mathbf{A}\mathbf{y}^* = \pm 2\rho(1-\rho).$ From the fact $\mathbf{x}^{*}{}'\mathbf{A}\mathbf{z}^* = \pm 2\rho(1+\rho)$ and Lemma 2.3 (a), we obtain that $scons(\mathbf{z}^*) - fcons(\mathbf{z}^*) = n/2,$ but it implies $\mathbf{1}'\mathbf{A}\mathbf{z}^* = 0$ by Lemma 2.3 (c). Hence $\tilde{\mathbf{X}}'\mathbf{A}\tilde{\mathbf{X}}$ has the form (3.1) and by Theorem 3.4, the thesis is true. ■

Basing on Theorems 3.3, 3.4 and Lemma 2.3, we can formulate the following theorem.

Theorem 3.6. If $\rho \in [0, 1/(n-2)]$, $n \equiv 0 \pmod 4$ and $\tilde{\mathbf{X}} = [\mathbf{1} \,|\, \mathbf{X}^*] \in M_{n\times 4}(\pm 1)$ is D–optimal in the class of designs $[\mathbf{1} \,|\, \mathbf{X}] \in M_{n\times 4}(\pm 1),\ rank([\mathbf{1} \,|\, \mathbf{X}]) = 4,$ then the design $\mathbf{X}^*$ is D–optimal in the class of designs $M_{n\times 3}(\pm 1).$

Theorems 3.5 and 3.6 can be use to find D–optimal designs in one of discussed classes of designs from the other one. For example, we known that the design $\hat{\mathbf{X}} = [\mathbf{1} \,|\, \hat{\mathbf{x}} \,|\, \hat{\mathbf{y}} \,|\, \hat{\mathbf{z}}]$ given by (1.2) is D–optimal in the class $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1), rank(\mathbf{X}) = 4$, so by Theorem 3.6 the design

$[\hat{\mathbf{x}} \,|\, \hat{\mathbf{y}} \,|\, \hat{\mathbf{z}}]$ is D–optimal in $M_{n\times 3}(\pm 1)$. Using theorems presented in this paper, we can get much more different examples of D–optimal designs. Moreover, the design $[\mathbf{1} \,|\, \hat{\mathbf{x}} \,|\, \hat{\mathbf{y}}]$ obtained from $\hat{\mathbf{X}}$ in the form (1.2) is the D–optimal design from Yeh and Lo Huang (2005) in the class of designs with the design matrix $[\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y}] \in M_{n\times 3}(\pm 1)$.

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