DOI: 10.1515/bile-2017-0008

Biometrical Letters
Vol. 54 (2017), No. 2, 137 - 154

Some D-optimal chemical balance weighing designs: theory and examples

Bronisław Ceranka[1], Małgorzata Graczyk[1]

[1]Department of Mathematical and Statistical Methods, Poznań University of Life Sciences,
Wojska Polskiego 28, 60-637 Poznań, Poland,
e-mail: bronicer@up.poznan.pl, magra@up.poznan.pl

SUMMARY

In this paper we study a certain kind of experimental designs called chemical balance weighing designs. We consider issues with regard to determining optimality conditions. We give new classes of designs in which we are able to determine an optimal design. Moreover, examples are given for the presented cases.

Key words: chemical balance weighing design, D-optimality

1. Introduction

Let us consider the class $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ of $n \times p$ design matrices $\mathbf{X}$ having entries $-1, 1$ or 0. Such a matrix is called the design matrix of a chemical balance weighing design (Banerjee, 1975). The problem considered is the determination of unknown measurements of objects $w_1, w_2,..., w_p$, when random observations $y_1, y_2,..., y_n$ are come from by the model $\mathbf{y} = \mathbf{Xw} + \mathbf{e}$, where $\mathbf{w} = (w_1, w_2,..., w_p)'$, $\mathbf{y} = (y_1, y_2,..., y_n)'$, $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$, $\mathbf{e} = (e_1, e_2,..., e_n)'$ is a random vector of errors with $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$, $\mathrm{Var}(\mathbf{e}) = \sigma^2\mathbf{I}_n$, as usual $\mathbf{0}_n$ is a vector of zeros, $\mathbf{I}_n$ is the identity matrix and σ^2 is a known scalar. The form of the variance matrix of errors means that the errors of measurements are uncorrelated and they have the same variances. If the matrix $\mathbf{X}$ is of full column rank, then the estimator of the vector $\mathbf{w}$ is given in the form $\hat{\mathbf{w}} = \mathbf{M}^{-1}\mathbf{X}'\mathbf{y}$, and its covariance matrix equals $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\mathbf{M}^{-1}$, where $\mathbf{M} = \mathbf{X}'\mathbf{X}$ is called the information matrix for the design $\mathbf{X}$.

An introduction to weighing designs and the basic problems related to them can be found in Jacroux et al. (1983), Sathe and Shenoy (1990) and the references given there. Certain kinds of weighing plans are used in spectroscopy (see Harwit and Sloane, 1979). Another important application of weighing designs is to 2^n fractional factorial designs (see Cheng, 2014). In a paper by Cheng and Kao (2015), these designs are employed in neuroimaging experiments where functional magnetic resonance imaging (fMRI) technology is used to obtain knowledge on how the brain reacts to certain mental stimuli. Another survey of common applications of weighing designs is given by Graczyk (2013).

Among many problems related to weighing designs, optimality criteria are frequently discussed. In the present paper, we consider D-optimal designs, i.e. optimal designs in which the generalized variance of parameter estimates is minimized. The design $\mathbf{X}_D$ is called D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if $\det\left(\mathbf{X}_D^{'}\mathbf{X}_D\right)=\max\left(\det(\mathbf{M}):\mathbf{X}\in\mathbf{\Phi}_{n\times p}\{-1,0,1\}\right)$. If $\det(\mathbf{M})$ attains the upper bound, then the design is called regular D-optimal. In other cases, such a design is simply called D-optimal. Each regular D-optimal design is D-optimal, although the converse need not hold. For a recent account of the theory of regular D-optimal chemical balance weighing designs we refer the reader to Masaro and Wong (2008), Neubauer and Pace (2010), Katulska and Smaga (2013), and Smaga (2014).

Although there is no shortage of theoretical work providing knowledge to guide the selection of optimal designs, we are not able to determine a regular D-optimal design for any combination of number of objects and number of measurements. Some solutions of this problem and some construction methods for D-optimal designs appear in the literature (see Ceranka and Graczyk, 2014b, 2015). Here, we study classes of design matrices that have not previously been considered, and give a new construction method for D-optimal designs. The idea is to take a regular D-optimal design and add one or more measurements to obtain a D-optimal design in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$, a class in which a regular D-optimal chemical balance weighing design does not exist.

We recall the definition of a D-optimal design and a theorem determining the parameters of a regular D-optimal design, given in Ceranka and Graczyk (2014a).

Definition 1. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ with the covariance matrix of errors $\sigma^2\mathbf{I}_n$ is regular D-optimal if $\det(\mathbf{M}) = m^p$, where m is the maximal number of elements equal to -1 and 1 in columns of $\mathbf{X}$.

Theorem 1. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ with the covariance matrix of errors $\sigma^2\mathbf{I}_n$ is regular D-optimal if and only if $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p$.

2. The main result

2.1. Admixing of one measurement

Let $\mathbf{X}_1 \in \mathbf{\Psi}_{(n-1)\times p}\{-1, 0, 1\}$ be the design matrix of a regular D-optimal chemical balance weighing design. Now, let us consider the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{x}_1' \end{bmatrix}, \tag{1}$$

where $\mathbf{x}_1$ is any $p\times 1$ vector of elements $-1, 1$ or 0, $\mathbf{x}_1'\mathbf{x}_1 = t_1$, $1 \le t_1 \le p$. Furthermore, we study the function $\det(\mathbf{M})$. According to Theorem 18.1.1 in Harville (1997), for $\mathbf{X}$ in the form (1), we have

$$\det(\mathbf{M}) = \det\left(\mathbf{X}_1'\mathbf{X}_1\right)\cdot\left(1 + \mathbf{x}_1'\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1}\mathbf{x}_1\right).$$

We are interested in determining the maximum of $\det(\mathbf{M})$ under a given matrix $\mathbf{X}_1$. We know that the function $\det(\mathbf{M})$ as a function of t_1 attains the maximum if and only if $t_1 = p$. Hence, we may state the following theorem:

Theorem 2. Any chemical balance weighing design $\mathbf{X}$ in the form (1) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ if and only if $\mathbf{x}_1'\mathbf{x}_1 = p$.

Definition 2. Any chemical balance weighing design $\mathbf{X}$ in the form (1) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if $\det(\mathbf{M}) = m^{p-1}(m+p)$.

Following Bulutoglu and Ryan (2009) we define the D-efficiency of the design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ as

$$\mathrm{D}_{eff}(\mathbf{X}) = \sqrt[p]{\frac{\det(\mathbf{X}'\mathbf{X})}{\max\limits_{\mathbf{Y}\in\mathbf{\Phi}_{n\times p}\{-1,0,1\}} \det(\mathbf{Y}'\mathbf{Y})}}.$$

For a D-optimal chemical balance weighing design $\mathbf{X}$ in the form (1),

$$\mathrm{D}_{eff}(\mathbf{X}) = \frac{m}{m+1}\sqrt[p]{\frac{m+p}{m}} < 1.$$

Example 1. We determine a D-optimal design in the class $\mathbf{X}\in\mathbf{\Phi}_{13\times 6}\{-1,0,1\}$. Let us consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1\in\mathbf{\Psi}_{12\times 6}\{-1,0,1\}$ in the form

$$\mathbf{X}_1' = \begin{bmatrix} 1 & -1 & 0 & -1 & -1 & 0 & -1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 & -1 & -1 & 0 & -1 & 1 & 0 & 1 & 1 \\ -1 & 0 & 1 & -1 & 0 & -1 & 1 & 0 & -1 & 1 & 0 & 1 \\ -1 & -1 & 0 & 1 & -1 & 0 & 1 & 1 & 0 & -1 & 1 & 0 \\ 0 & -1 & -1 & 0 & 1 & -1 & 0 & 1 & 1 & 0 & -1 & 1 \\ -1 & 0 & -1 & -1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & -1 \end{bmatrix}.$$

Then, the matrix $\mathbf{X}\in\mathbf{\Phi}_{13\times 6}\{-1,0,1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & & & \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9758$.

2.2. Admixing of two measurements

Let $\mathbf{X}_1\in\mathbf{\Gamma}_{(n-2)\times p}\{-1,0,1\}$ be the design matrix of a regular D-optimal chemical balance weighing design. We study the design matrix $\mathbf{X}\in\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ given as

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{x}_1^{'} \\ \mathbf{x}_2^{'} \end{bmatrix}, \tag{2}$$

where $\mathbf{x}_1, \mathbf{x}_2$ are vectors of elements $-1, 1$ or 0, $\mathbf{x}_\tau^{'}\mathbf{x}_\tau = t_\tau$, $1 \le t_\tau \le p$, $\mathbf{x}_\tau^{'}\mathbf{x}_\kappa = \mathbf{x}_\kappa^{'}\mathbf{x}_\tau = u_{\tau\kappa}$, $\tau, \kappa = 1{,}2$. Our goal is to determine the maximum of the function $\det(\mathbf{M})$ under the given matrix $\mathbf{X}_1$. Applying the equality given in Theorem 18.1.1 in Harville (1997) to $\mathbf{X}$ in the form (2.2), we obtain

$$\begin{aligned} \det(\mathbf{M}) &= \det\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)\cdot \det\left(\mathbf{I}_2 + \begin{bmatrix} \mathbf{x}_1^{'} \\ \mathbf{x}_2^{'} \end{bmatrix}\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)^{-1}\begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}\right). \\ &= m^{p-2}\left((m+t_1)(m+t_2) - u_{12}^2\right) \end{aligned}$$

The maximum of $\det(\mathbf{M})$ is attained if and only if the maximum of $m + t_1$, $m + t_2$ and the minimum of u_{12}^2 are simultaneously attained. We determine the maximum of $\det(\mathbf{M})$ in the class $\mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$, thus $t_\tau = p$, $\tau = 1{,}2$, and consequently, $\det(\mathbf{M}) = m^{p-2}\left((m+p)^2 - u_{12}^2\right)$. Let us note that u_{12} is the scalar product of two rows of the matrix having elements $-1, 1, 0$, and $u_{12} = 0$ if and only if p is even. In this case, $\det(\mathbf{M}) = m^{p-2}(m+p)^2$. When p is odd, the condition $u_{12} = 0$ is never fulfilled. For an odd number of objects, the maximum of $\det(\mathbf{M})$ is attained if and only if u_{12} takes the smallest value $+1$ or -1. Then $\det(\mathbf{M}) = m^{p-2}\left((m+p)^2 - 1\right)$. We may thus state the following theorem:

Theorem 3. Any chemical balance weighing design $\mathbf{X}$ in the form (2) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ if and only if $\mathbf{x}_\tau^{'}\mathbf{x}_\tau = p$ and

$$u_{12} = \begin{cases} 0, & \text{when } p \text{ is even} \\ \pm 1, & \text{when } p \text{ is odd} \end{cases}, \quad \tau = 1{,}2.$$

Definition 3. Any chemical balance weighing design $\mathbf{X}$ in the form (2) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ if

$$\det(\mathbf{M}) = \begin{cases} m^{p-2}(m+p)^2, & \text{when } p \text{ is even} \\ m^{p-2}\left((m+p)^2 - 1\right), & \text{when } p \text{ is odd} \end{cases}.$$

It should be noted that, for the D-optimal chemical balance weighing design $\mathbf{X}$ in the form (2),

$$\mathrm{D}_{eff}(\mathbf{X}) = \frac{m^{\frac{p-2}{2}}}{m+2} \cdot \begin{cases} \sqrt[p]{(m+p)^2}, & \text{when } p \text{ is even} \\ \sqrt[p]{(m+p)^2 - 1}, & \text{when } p \text{ is odd} \end{cases}.$$

Example 2. To determine a D-optimal design in the class $\mathbf{X} \in \mathbf{\Phi}_{6\times4}\{-1, 0, 1\}$ we consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Gamma}_{4\times4}\{-1, 0, 1\}$ given in the form

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{bmatrix}.$$

Then the matrix $\mathbf{X} \in \mathbf{\Phi}_{6\times4}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & \mathbf{X}_1 & & \\ 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \end{bmatrix}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9428$.

Example 3. To determine a D-optimal design in the class $\mathbf{X} \in \mathbf{\Phi}_{30\times7}\{-1, 0, 1\}$, we take the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Gamma}_{28\times7}\{-1, 0, 1\}$ in the form $\mathbf{X}_1' = [\mathbf{X}_{11} \quad \mathbf{X}_{12} \quad \mathbf{X}_{13}]$, where

$$\mathbf{X}_{11} = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & -1 & 1 & 1 \end{bmatrix}, \quad \mathbf{X}_{12} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & 1 & -1 \end{bmatrix}$$

$$\mathbf{X}_{13}=\begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \end{bmatrix}.$$

Then the matrix $\mathbf{X}\in\mathbf{\Phi}_{30\times 7}\{-1,0,1\}$ given as

$$\mathbf{X}=\begin{bmatrix} & & & \mathbf{X}_1 & & & \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & 1 & 1 \end{bmatrix}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X})=0.9945$.

2.3. Admixing of three measurements

Let $\mathbf{X}_1\in\mathbf{\Xi}_{(n-3)\times p}\{-1,0,1\}$ be the design matrix of a regular D-optimal chemical balance weighing design. Now, we consider the design matrix $\mathbf{X}\in\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form

$$\mathbf{X}=\begin{bmatrix}\mathbf{X}_1\\ \mathbf{x}_1^{'}\\ \mathbf{x}_2^{'}\\ \mathbf{x}_3^{'}\end{bmatrix}, \tag{3}$$

where $\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3$ are some vectors of elements $-1,1$ or 0, $\mathbf{x}_\tau^{'}\mathbf{x}_\tau=t_\tau$, $\mathbf{x}_\tau^{'}\mathbf{x}_\kappa=\mathbf{x}_\kappa^{'}\mathbf{x}_\tau=u_{\tau\kappa}$, $1\le t_\tau\le p$, $1\le\tau<\kappa\le 3$. Following the condition given in Theorem 18.1.1 in Harville (1997),

$$\det(\mathbf{M})=\det\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)\cdot\det\left(\mathbf{I}_3+\begin{bmatrix}\mathbf{x}_1^{'}\\ \mathbf{x}_2^{'}\\ \mathbf{x}_3^{'}\end{bmatrix}\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)^{-1}\begin{bmatrix}\mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3\end{bmatrix}\right),$$

for $\mathbf{X}$ in the form (3) we obtain $\det(\mathbf{M})=\det\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)\cdot\det(\mathbf{\Omega})$, where

$$\mathbf{\Omega} = \frac{1}{m}\begin{bmatrix} m+t_1 & u_{12} & u_{13} \\ u_{12} & m+t_2 & u_{23} \\ u_{13} & u_{23} & m+t_3 \end{bmatrix}.$$

Now, we are interested in determining the maximum of the function $\det(\mathbf{M})$. Because we determine the maximum in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$, it is obvious that $t_\tau = p$, $\tau = 1,2,3$, and furthermore, $\det(\mathbf{M}) = m^{p-3}\cdot\det(\mathbf{I}_3 + \mathbf{A}'\mathbf{A})$, where $\mathbf{A} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3]$. From the construction of the matrix $\mathbf{X}$ in the form (3) it follows that the maximum of $\det(\mathbf{M})$ is attained if and only if $\det(\mathbf{A}'\mathbf{A})$ takes the largest value. Here we state a lemma given in Payne (1974), which provides the basis for many of the computations in this section.

Lemma 1. Let $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$ be three $n_0 \times 1$ column vectors of ± 1's. If $\mathbf{B}$ is the $n \times 3$ matrix whose columns are $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$ in some order, then $\det(\mathbf{B}'\mathbf{B})$ is maximal if and only if the following conditions are satisfied:
(i) If $n_0 \equiv 0(\mathrm{mod}\ 4)$, the dot product $\mathbf{c}_s \cdot \mathbf{c}_t = 0$ for $1 \le s < t \le 3$.
(ii) If $n_0 + 2 \equiv 0(\mathrm{mod}\ 4)$, then $\mathbf{c}_s \cdot \mathbf{c}_t = \pm 2$ or 0 for $1 \le s < t \le 3$, with 0 occurring twice and ± 2 occurring once.
(iii) If $n_0 + 1 \equiv 0(\mathrm{mod}\ 4)$, then $\mathbf{c}_s \cdot \mathbf{c}_t = \pm 1$ for $1 \le s < t \le 3$, with $+1$ occurring an even number of times.
(iv) If $n_0 + 3 \equiv 0(\mathrm{mod}\ 4)$, then $\mathbf{c}_s \cdot \mathbf{c}_t = \pm 1$ for $1 \le s < t \le 3$, with -1 occurring an even number of times.

Putting $n_0 = p$ and $\mathbf{c}_s = \mathbf{x}_s$, $s = 1,2,3$, we obtain that if $p \equiv 0\,(\mathrm{mod}\ 4)$, then the maximum of $\det(\mathbf{M})$ is attained if and only if $u_{\tau\kappa} = 0$ for $1 \le \tau < \kappa \le 3$ and then, $\det(\mathbf{M}) = m^{p-3}(m+p)^3$. If $p + 2 \equiv 0\,(\mathrm{mod}\ 4)$, then the maximum of $\det(\mathbf{M})$ is attained if and only if $|u_{\tau\kappa}| = 2$ or 0 for $1 \le \tau < \kappa \le 3$, with 0 occurring twice and ± 2 occurring once, and $\det(\mathbf{M}) = m^{p-3}\left((m+p)^3 - 4(m+p)\right)$. If $p + 1 \equiv 0\,(\mathrm{mod}\ 4)$, then the maximum of $\det(\mathbf{M})$ is attained if and only if $u_{\tau\kappa} = \pm 1$ and $\prod u_{\tau\kappa} = -1$ for $1 \le \tau < \kappa \le 3$. Here, $\det(\mathbf{M}) = m^{p-3}\left((m+p)^3 - 3(m+p) - 2\right)$. If $p + 3 \equiv 0\,(\mathrm{mod}\ 4)$, then the maximum of $\det(\mathbf{M})$ is attained if and only if $u_{\tau\kappa} = \pm 1$ and $\prod u_{\tau\kappa} = 1$ for $1 \le \tau < \kappa \le 3$.

Hence $\det(\mathbf{M}) = m^{p-3}\left((m+p)^3 - 3(m+p) + 2\right)$. We may thus state the following theorem:

Theorem 4. Any chemical balance weighing design $\mathbf{X}$ in the form (3) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if and only if $\mathbf{x}_\tau^{'}\mathbf{x}_\tau = p$ for $\tau = 1,2,3$, and for $\tau,\kappa,\xi = 1,2,3,\ \tau \neq \kappa \neq \xi$, we have

(i) when $p \equiv 0 \pmod 4$, $u_{\tau\kappa} = 0$,

(ii) when $p+2 \equiv 0 \pmod 4$, $u_{\tau\kappa} = \pm 2$ and $u_{\tau\xi} = u_{\kappa\xi} = 0$,

(iii) when $p+1 \equiv 0 \pmod 4$, $u_{\tau\kappa} = \pm 1$ and $\prod u_{\tau\kappa} = -1$,

(iv) when $p+3 \equiv 0 \pmod 4$, $u_{\tau\kappa} = \pm 1$ and $\prod u_{\tau\kappa} = 1$.

Definition 4. Any chemical balance weighing design $\mathbf{X}$ in the form (3) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if

$$\det\left(\mathbf{X}^{'}\mathbf{X}\right) = \begin{cases} m^{p-3}(m+p)^3, & \text{when} \quad p \equiv 0 \pmod 4 \\ m^{p-3}\left((m+p)^3 - 4(m+p)\right), & \text{when} \quad p+2 \equiv 0 \pmod 4 \\ m^{p-3}\left((m+p)^3 - 3(m+p) - 2\right), & \text{when} \quad p+1 \equiv 0 \pmod 4 \\ m^{p-3}\left((m+p)^3 - 3(m+p) + 2\right), & \text{when} \quad p+3 \equiv 0 \pmod 4 \end{cases}.$$

Let us note that for the D-optimal chemical balance weighing design $\mathbf{X}$ in the form (2.3)

$$\mathrm{D}_{eff}(\mathbf{X}) = \frac{m^{\frac{p-3}{p}}}{m+3} \cdot \begin{cases} \sqrt[p]{(m+p)^3}, & \text{when } p \equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^3 - 4(m+p)}, & \text{when } p+2 \equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^3 - 3(m+p) - 2}, & \text{when } p+1 \equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^3 - 3(m+p) + 2}, & \text{when } p+3 \equiv 0 \pmod 4 \end{cases}.$$

Example 4. We determine unknown measurements of $p = 4$ objects $\left(p \equiv 0 \pmod 4\right)$ in $n = 15$ measurements according to the D-optimality criterion. We consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Xi}_{12\times 4}\{-1,0,1\}$ given in the form

$$\mathbf{X}_1' = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 0 & -1 & 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & -1 & -1 & -1 & -1 & 0 & -1 & 1 & -1 & 1 & 0 & 0 \\ -1 & 1 & -1 & -1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & -1 \end{bmatrix}.$$

From this, the matrix $\mathbf{X} \in \mathbf{\Phi}_{15\times 4}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \end{bmatrix}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9882$.

Example 5. In an attempt to determine a D-optimal design for $p = 6$ objects $(p + 2 \equiv 0 \pmod 4)$ in $n = 9$ measurements, i.e. in the class $\mathbf{X} \in \mathbf{\Phi}_{9\times 6}\{-1, 0, 1\}$, we take the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Xi}_{6\times 6}\{-1, 0, 1\}$ in the form

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 0 & -1 & -1 & 0 & -1 \\ -1 & 1 & 0 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 & -1 & -1 \\ -1 & 0 & -1 & 1 & 0 & -1 \\ -1 & -1 & 0 & -1 & 1 & 0 \\ 0 & -1 & -1 & 0 & -1 & 1 \end{bmatrix}.$$

Then $\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & & & \\ 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 \end{bmatrix} \in \mathbf{\Phi}_{9\times 6}\{-1, 0, 1\}$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.8974$.

Example 6. To determine a D-optimal design in the class $\mathbf{X} \in \mathbf{\Phi}_{7\times 3}\{-1, 0, 1\}$, i.e. for $p = 3$ objects $(p + 1 \equiv 0 \pmod 4)$ in $n = 7$ measurements, we consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Xi}_{4\times 3}\{-1, 0, 1\}$ in the form

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{bmatrix}.$$

Then the matrix $\mathbf{X} \in \mathbf{\Phi}_{7\times 3}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & \mathbf{X}_1 & \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{bmatrix}$$

is D-optimal, and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9771$.

Example 7. We are interested in determining a D-optimal design for $p = 5$ objects $(p + 3 \equiv 0 \pmod 4)$ in $n = 28$ measurements, i.e. in the class $\mathbf{X} \in \mathbf{\Phi}_{28\times 5}\{-1, 0, 1\}$. Let us consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Xi}_{25\times 5}\{-1, 0, 1\}$ in the form

$$\mathbf{X}_1 = \begin{bmatrix} \mathbf{X}_{11} \\ \mathbf{X}_{12} \end{bmatrix}, \text{ where } \mathbf{X}_{11}^{'} = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & -1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & -1 \\ 0 & -1 & 1 & 0 & 0 & 1 & -1 & 1 & 0 & 1 \\ 0 & 0 & -1 & 1 & -1 & 0 & 1 & 0 & 1 & 1 \end{bmatrix},$$

$$\mathbf{X}_{12}^{'} = \begin{bmatrix} 1 & 0 & -1 & -1 & -1 & 0 & -1 & 0 & -1 & 0 & -1 & 0 & -1 & 0 & 0 \\ -1 & 1 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & -1 & -1 \\ -1 & -1 & 1 & 0 & -1 & -1 & 0 & 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & -1 \\ 0 & -1 & -1 & -1 & 1 & -1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}.$$

Then the matrix $\mathbf{X} \in \mathbf{\Phi}_{28\times 5}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & & \\ 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 \end{bmatrix}$$

is D-optimal, and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9875$.

2.4. Admixing of four measurements

Let $\mathbf{X}_1 \in \mathbf{\Theta}_{(n-4)\times p}\{-1, 0, 1\}$ be the design matrix of a regular D-optimal chemical balance weighing design. Next, suppose that the matrix $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ is of the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{x}_1^{'} \\ \mathbf{x}_2^{'} \\ \mathbf{x}_3^{'} \\ \mathbf{x}_4^{'} \end{bmatrix}, \tag{4}$$

where $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$ are some vectors of elements $-1, 1$ or 0, $\mathbf{x}_\tau^{'}\mathbf{x}_\kappa = \mathbf{x}_\kappa^{'}\mathbf{x}_\tau = u_{\tau\kappa}$, $1 \le \tau < \kappa \le 4$. According the equality given in Theorem 18.1.1 in Harville (1997),

$$\det(\mathbf{M}) = \det\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)\cdot \det\left(\mathbf{I}_4 + \begin{bmatrix} \mathbf{x}_1^{'} \\ \mathbf{x}_2^{'} \\ \mathbf{x}_3^{'} \\ \mathbf{x}_4^{'} \end{bmatrix}\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)^{-1}\begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_4 \end{bmatrix}\right),$$

for $\mathbf{X}$ in the form (4) we have $\det(\mathbf{M}) = \det\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)\cdot \det(\mathbf{T})$, where

$$\mathbf{T} = \frac{1}{m}\begin{bmatrix} m+t_1 & u_{12} & u_{13} & u_{14} \\ u_{12} & m+t_2 & u_{23} & u_{24} \\ u_{13} & u_{23} & m+t_3 & u_{34} \\ u_{14} & u_{24} & u_{34} & m+t_4 \end{bmatrix}.$$

The question becomes how to determine the maximum of $\det(\mathbf{M})$ under a given matrix $\mathbf{X}_1$ of a regular D-optimal design. We determine the maximum in the class

$\mathbf{\Phi}_{n\times p}\{-1,0,1\}$, thus $t_\tau = p$, $\tau = 1,2,3,4$, and then $\det(\mathbf{M}) = m^{p-4}\cdot\det(\mathbf{I}_4 + \mathbf{C}'\mathbf{C})$, where $\mathbf{C} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \mathbf{x}_4]$. From the construction of the matrix $\mathbf{X}$ in the form (4), the problem of determining the maximum of $\det(\mathbf{M})$ is now reduced to determining the maximum of $\det(\mathbf{C}'\mathbf{C})$. Payne (1974) proved the following lemma.

Lemma 2. Let $\mathbf{D}$ be an $n_0 \times 4$ matrix of ± 1's, where $n_0 \geq 4$. Then $\det(\mathbf{D}'\mathbf{D})$ is maximal if and only if each three columns of $\mathbf{D}$ form $\mathbf{D}_1$ for which $\det(\mathbf{D}_1'\mathbf{D}_1)$ is maximal.

Taking $n_0 = p$ we obtain that in the case $p \equiv 0 \pmod 4$, the condition determining a D-optimal design is the same as in subsection 2.3. Furthermore, $\det(\mathbf{M}) = m^{p-4}(m+p)^4$. The computations for the case $p+2 \equiv 0 \pmod 4$ indicate that the maximum of $\det(\mathbf{M})$ is attained if and only if $|u_{\tau\kappa}| = 2$ or 0 for $1 \leq \tau < \kappa \leq 4$, with ± 2 occurring twice and 0 occurring four times. In that case $\det(\mathbf{M}) = m^{p-4}\left((m+p)^4 - 8(m+p)^2 + 16\right)$. Furthermore, if $p+1 \equiv 0 \pmod 4$, exploring all possibilities of combinations of $u_{\tau\kappa}$ for $1 \leq \tau < \kappa \leq 4$, we obtain that the maximum of $\det(\mathbf{M})$ is attained if and only if $u_{\tau\kappa} = \pm 1$ and, that's more $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\xi} = -1$ and $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\eta}u_{\xi\eta} = 1$, $\tau,\kappa,\xi,\eta = 1,2,3,4,\ \tau \neq \kappa \neq \xi \neq \eta$. In that case $\det(\mathbf{M}) = m^{p-4}\left((m+p)^4 - 6(m+p)^2 - 8(m+p) - 3\right)$. If $p+3 \equiv 0 \pmod 4$, then a check of all possible combinations of $u_{\tau\kappa}$, $1 \leq \tau < \kappa \leq 4$, reveals that the maximum of $\det(\mathbf{M})$ is attained if and only if $u_{\tau\kappa} = \pm 1$ and, additionally, $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\xi} = 1$ and $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\eta}u_{\xi\eta} = 1$ for $\tau,\kappa,\xi,\eta = 1,2,3,4,\ \tau \neq \kappa \neq \xi \neq \eta$. Hence $\det(\mathbf{X}'\mathbf{X}) = m^{p-4}\left((m+p)^4 - 6(m+p)^2 + 8(m+p) - 3\right)$. In summary, we may formulate the following theorem:

Theorem 5. Any chemical balance weighing design $\mathbf{X}$ in the form (4) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if and only if $\mathbf{x}_\tau'\mathbf{x}_\tau = p$ and for $\tau,\kappa,\xi,\eta = 1,2,3,4,\ \tau \neq \kappa \neq \xi \neq \eta$,

(i) when $p \equiv 0 \pmod 4$, $u_{\tau\kappa} = 0$,

(ii) when $p+2 \equiv 0 \pmod 4$, $u_{\tau\kappa} = u_{\xi\eta} = \pm 2$ and the others are 0's,

(iii) when $p+1 \equiv 0 \pmod 4$, $u_{\tau\kappa} = \pm 1$, $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\xi} = -1$ and $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\eta}u_{\xi\eta} = 1$,

(iv) when $p+3 \equiv 0 \pmod 4$, $u_{\tau\kappa} = \pm 1$, $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\xi} = 1$ and $u_{\tau\kappa}u_{\tau\xi}u_{\kappa\eta}u_{\xi\eta} = 1$.

Definition 5. Any chemical balance weighing design $\mathbf{X}$ in the form (4) is D-optimal in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ if and only if

$$\det\left(\mathbf{X}'\mathbf{X}\right)=\begin{cases} m^{p-4}(m+p)^4, & \text{when} \quad p\equiv 0 \pmod 4 \\ m^{p-4}\left((m+p)^4-8(m+p)^2+16\right), & \text{when} \quad p+2\equiv 0 \pmod 4 \\ m^{p-4}\left((m+p)^4-6(m+p)^2-8(m+p)-3\right), & \text{when} \quad p+1\equiv 0 \pmod 4 \\ m^{p-4}\left((m+p)^4-6(m+p)^2+8(m+p)-3\right), & \text{when} \quad p+3\equiv 0 \pmod 4 \end{cases}$$

Let us note that, for a D-optimal chemical balance weighing design $\mathbf{X}$ in the form (4),

$$\mathrm{D}_{eff}\left(\mathbf{X}\right)=\frac{m^{\frac{p-4}{4}}}{m+4}\cdot\begin{cases} \sqrt[p]{(m+p)^4}, & \text{when } p\equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^4-8(m+p)^2+16}, & \text{when } p+2\equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^4-6(m+p)^2-8(m+p)-3}, & \text{when } p+1\equiv 0 \pmod 4 \\ \sqrt[p]{(m+p)^4-6(m+p)^2+8(m+p)-3}, & \text{when } p+3\equiv 0 \pmod 4 \end{cases}.$$

Example 8. To determine an optimal design for $p=8$ objects $(p\equiv 0 \pmod 4))$ in $n=16$ measurements, i.e. in the class $\mathbf{X}\in\mathbf{\Phi}_{16\times 8}\{-1,0,1\}$, we consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1\in\mathbf{\Theta}_{12\times 8}\{-1,0,1\}$ given in the form

$$\mathbf{X}_1'=\begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 0 & 1 & 0 & 0 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 0 & 0 & 1 & 0 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 0 & -1 & 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & -1 & -1 & -1 & -1 & 0 & -1 & 1 & -1 & 1 & 0 & 0 \\ -1 & 1 & -1 & -1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 & -1 & -1 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}.$$

Then the matrix $\mathbf{X}\in\mathbf{\Phi}_{16\times 8}\{-1,0,1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & & \mathbf{X}_1 & & & & \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 \end{bmatrix}$$

is D-optimal. Here $\mathrm{D}_{eff}(\mathbf{X}) = 0.9515$.

Example 9. To determine a D-optimal design for $p = 6$ objects $(p + 2 \equiv 0 \,(\mathrm{mod}\, 4))$ in $n = 28$ measurements, i.e. in the class $\mathbf{X} \in \mathbf{\Phi}_{28\times6}\{-1, 0, 1\}$, we take the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Theta}_{24\times6}\{-1, 0, 1\}$ given in the form

$$\mathbf{X}_1 = \begin{bmatrix} \mathbf{X}_1^* & \mathbf{1}_{10} \\ -\mathbf{X}_1^* & -\mathbf{1}_{10} \\ \mathbf{1}_2\mathbf{1}_5' & \mathbf{0}_2 \\ -\mathbf{1}_2\mathbf{1}_5' & \mathbf{0}_2 \end{bmatrix}, \text{ where } (\mathbf{X}_1^*)' = \begin{bmatrix} 1 & 1 & 0 & -1 & 1 & 1 & -1 & 0 & -1 & -1 \\ 1 & 0 & -1 & 1 & 0 & -1 & 1 & -1 & 1 & -1 \\ 0 & -1 & 1 & 1 & -1 & 1 & 0 & -1 & -1 & 1 \\ -1 & 1 & 1 & 0 & -1 & -1 & -1 & 1 & 1 & 0 \\ -1 & -1 & -1 & -1 & 1 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

Then

$$\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & & & \\ 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 \end{bmatrix} \in \mathbf{\Phi}_{28\times6}\{-1, 0, 1\}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9940$.

Example 10. In order to determine a D-optimal design in the class $\mathbf{X} \in \mathbf{\Phi}_{18\times7}\{-1, 0, 1\}$, i.e. for $p = 7$ objects $(p + 1 \equiv 0 \,(\mathrm{mod}\, 4))$ in $n = 18$ measurements, we consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Theta}_{14\times7}\{-1, 0, 1\}$ given as

$$\mathbf{X}_1^{'} = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 1 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & -1 & -1 & -1 \\ 0 & 1 & 0 & 0 & -1 & 1 & 1 & 0 & -1 & -1 & 1 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 & 0 & 1 & -1 & 0 & -1 & 0 & -1 & 1 & -1 & 0 \\ 1 & -1 & 0 & 1 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & -1 \\ 1 & 1 & -1 & 0 & 1 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}.$$

Then the matrix $\mathbf{X} \in \mathbf{\Phi}_{18\times 7}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & & \mathbf{X}_1 & & & \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix}$$

is D-optimal and $\mathrm{D}_{eff}(\mathbf{X}) = 0.9508$.

Example 11. To determine an optimal design for $p = 5$ objects $(p + 3 \equiv 0 \pmod 4)$ in $n = 24$ measurements, i.e. in the class $\mathbf{X} \in \mathbf{\Phi}_{24\times 5}\{-1, 0, 1\}$, let us consider the regular D-optimal chemical balance weighing design $\mathbf{X}_1 \in \mathbf{\Theta}_{20\times 5}\{-1, 0, 1\}$ given by $\mathbf{X}_1^{'} = \begin{bmatrix}\mathbf{X}_{11} & \mathbf{X}_{12}\end{bmatrix}$, where

$$\mathbf{X}_{11} = \begin{bmatrix} 0 & 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 \\ -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & 1 \\ 1 & -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 \\ 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 \end{bmatrix},$$

$$\mathbf{X}_{12} = \begin{bmatrix} -1 & -1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 0 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 0 & 1 & 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 0 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 0 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 \end{bmatrix}.$$

From the above, it follows that the matrix $\mathbf{X} \in \mathbf{\Phi}_{19\times 7}\{-1, 0, 1\}$ given as

$$\mathbf{X} = \begin{bmatrix} & & \mathbf{X}_1 & & \\ 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \end{bmatrix}$$

is D-optimal, $\mathrm{D}_{eff}(\mathbf{X}) = 0.9926$.

3. Conclusions

Although a regular D-optimal design is the most desirable, in some classes such a design does not exist. These cases are considered here, and are compared from the point of view of efficiency. According to the literature, the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1, 0, 1\}$ is regular D-optimal if and only if $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p$. Obviously, $1 \le m \le n$ and m is interpreted as the maximal number of non-zero elements in columns of the design matrix. From the practical point of view, this number indicates how many times each object is taken into account in measurement combinations. Sometimes it is difficult to include all objects in each measurement operation. For this reason, in many applications the case $1 \le m < n$ is considered. Evidently, a larger value of m results in a smaller variance of estimators on unknown measurements of objects. Taking into account these issues, in the present work, m is not fixed. However, all objects are included in measurement combinations in admixed measurements in order to obtain a D-optimal design.

REFERENCES

Banerjee K.S. (1975): Weighing Designs For Chemistry, Medicine, Economics, Operations Research, Statistics. Marcel Dekker Inc., New York.

Bulutoglu D.A., Ryan K.J. (2009): D-optimal and near D-optimal 2k fractional factorial designs of resolution V, Journal of Statistical Planning and Inference, 139: 16-22.

Ceranka B., Graczyk M. (2014a): The problem of D-optimality in some experimental designs. International Journal of Mathematics and Computer Application Research 4: 11-18.

Ceranka B., Graczyk M. (2014b): Construction of the regular D-optimal weighing designs with non-negative correlated errors. Colloquium Biometricum 44: 43-56.

Ceranka B., Graczyk M. (2015): Relations between ternary designs and D-optimal weighing designs with non-negative correlated errors. Colloquium Biometricum 145: 23-34.

Cheng C.S. (2014): Optimal biased weighing designs and two-level main-effect plans. Journal of Statistical Theory and Practice 8: 83-99.

Cheng C.S., Kao M.H. (2015): Optimal experimental designs for fMRI via circulant biased weighing designs. The Annals of Statistics 43: 2565-2587.

Graczyk M. (2013): Some applications of weighing designs. Biometrical Letters 50(1): 15-26.

Harville D.A. (1997): Matrix Algebra from a Statistician's Perspective. Springer-Verlag, New York Inc.

Harwit M., Sloane N.J.A. (1979): Hadamard transform optics. New York, Academic Press.

Jacroux M., Wong C.S., Masaro J.C. (1983). On the optimality of chemical balance weighing designs. Journal of Statistical Planning and Inference 8: 231-240.

Katulska K., Smaga Ł. (2013). A note on D-optimal chemical balance weighing designs and their applications. Colloquium Biometricum 43: 37-45.

Masaro J., Wong C.S. (2008): D-optimal designs for correlated random vectors. Journal of Statistical Planning and Inference 138: 4093-4106.

Neubauer G.N., Pace R.G. (2010): D-optimal (0,1)-weighing designs for eight objects. Linear Algebra and its Applications 432: 2634-2657.

Payne S.E. (1974): On maximizing det(A^TA). Discrete Mathematics 10: 145-458.

Sathe Y.S., Shenoy R.G. (1990): Construction method for some A- and D-optimal weighing designs when $N \equiv 3(\mathrm{mod}\,4)$. Journal of Statistical Planning and Inference 24: 369-375.

Smaga Ł. (2014): Necessary and sufficient conditions in the problem of D-optimal weighing designs with autocorrelated errors. Statistics and Probability Letters 92: 12-16.