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D-optimal chemical balance weighing designs with positively correlated errors: part I

Małgorzata Graczyk, Bronisław Ceranka

Department of Mathematical and Statistical Methods, Poznań University of Life Sciences
Wojska Polskiego 28, 60-638 Poznań, Poland, e-mails: malgorzata.graczyk@up.poznan.pl,
bronislaw.ceranka@up.poznan.pl

SUMMARY

In this paper, the problem of indicating chemical balance weighing designs satisfying the criterion of D-optimality is considered. Moreover, we study such designs under the assumption that the measurements are equally positively correlated and they have the same variances. We formulate a method to add at most four runs to a regular D-optimal chemical balance weighing design to obtain a highly D-efficient chemical balance weighing deign.

Key words: chemical balance weighing design, D-optimality, plan of experiment

1. Introduction

The planning of experiments is a very important area of mathematical statistics. Among many conditions determining the best experimental plan, it is very important to establish the optimality criterion. The choice of this criterion influences the form of the estimators to be determined, because optimality criteria are functions of the information matrix. In this paper we determine the best experimental plan for a chemical balance weighing design. Such designs can be applied in agriculture, economics, optics, and many other fields.

Let us consider the matrix $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$, where $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ denotes the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$, $i = 1,2,\dots,n$, $j = 1,2,\dots,p$, of known elements equal to –1, 0 or 1. Such a matrix is called the matrix of a chemical balance weighing design. The results of n measurement operations of p objects

will fit to a linear model $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where $\mathbf{y}$ is an $n \times 1$ random vector of observations, $\mathbf{w}$ is a $p \times 1$ vector of uknown measurements of objects, and $\mathbf{e}$ is an $n \times 1$ random vector of errors with E($\mathbf{e}$)=$\mathbf{0}_n$ and Var($\mathbf{e}$)=$\sigma^2\mathbf{G}$, where $\mathbf{0}_n$ is the $n \times 1$ vector with zero elements everywhere, σ^2 is a constant, and $\mathbf{G}$ is a known $n \times n$ positive definite matrix of the form

$$\mathbf{G} = (\mathbf{1} - \boldsymbol{\rho})\mathbf{I}_{\boldsymbol{n}} + \boldsymbol{\rho}\mathbf{1}_{\boldsymbol{n}}\mathbf{1}_{\boldsymbol{n}}', \quad \mathbf{0} < \boldsymbol{\rho} < \mathbf{1}. \tag{1.1}$$

The form of the matrix $\mathbf{G}$ indicates that the measurement errors are equally positively correlated. For the estimation of $\mathbf{w}$ we use the normal equations $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}\mathbf{w} = \mathbf{X}'\mathbf{G}^{-1}\boldsymbol{y}$. If the matrix $\mathbf{X}$ is of full column rank, then the generalized least squares estimator of $\mathbf{w}$ is given by $\widehat{\mathbf{w}} = (\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{G}^{-1}\boldsymbol{y}$ and $\mathrm{Var}(\widehat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}$. The matrix $\mathbf{M} = \mathbf{X}'\mathbf{G}^{-1}\mathbf{X}$ is called the information matrix of the design $\mathbf{X}$.

In the literature, several optimality criteria, minimizing certain functions of the matrix $\mathbf{M}$, are considered. One of them is D-optimality. We say that the design $\mathbf{X}_\mathrm{D}$ is D-optimal in the class of all possible design matrices $\mathbf{X} \in \boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$ if

$$\det\left(\mathbf{X}_\mathbf{D}'\mathbf{G}^{-1}\mathbf{X}_\mathbf{D}\right) = \boldsymbol{max}\left\{\det\left(\mathbf{M}^{-1}\right): \mathbf{X} \in \boldsymbol{\Phi}_{\boldsymbol{n}\times\boldsymbol{p}}\{-\mathbf{1},\mathbf{0},\mathbf{1}\}\right\} \tag{1.2}$$

Under the assumption that the matrix $\mathbf{G}$ is of the form (1.1), Ceranka and Graczyk (2014) give conditions determining a regular D-optimal chemical balance weighing design, as well as examples of the construction of such designs based on the incidence matrices of balanced incomplete block designs. Here, we recall the definition and theorem concerning the regular D-optimal design given in the aforementioned paper for this particular case. Let $m = max\{m_1, m_2, \ldots, m_p\}$, where m_j, $j = 1,2,\ldots,p$, represents the number of elements equal to –1 or 1 in the j^{th} column of $\mathbf{X} \in \boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$.

Definition 1.1. Any chemical balance weighing design $\mathbf{X} \in \boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$ with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is regular D-optimal if and only if $\det(\mathbf{M}) = \left(\frac{m}{1-\rho}\right)^p$.

Let us note that a regular D-optimal design is D-optimal, whereas the inverse need not hold.

Theorem 1.1. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is regular D-optimal if and only if $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p$ and $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$ if $0 < \rho < 1$.

The condition $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$ means that in each column of $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ the numbers of elements equal to -1 and 1 should be the same. Although there is no shortage of theoretical works providing knowledge to aid the selection of optimal designs, we are able to determine a regular D-optimal design for any combination of numbers of measurements and objects. Some solutions to this problem and some methods of construction of D-optimal chemical balance weighing designs appear in the literature; see Ceranka and Graczyk (2014, 2015a, 2015b, 2016, 2018). 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 of this work is to expand the design matrix of a regular D-optimal chemical balance weighing design and add $s = 1,2$ measurements in order to obtain the design matrix of a D-optimal chemical balance weighing design in the class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$, a class in which no regular D-optimal chemical balance weighing design exists.

An important issue here is the efficiency of a chemical balance weighing design with $s = 1,2$ additional measurements. Following the definition of Bulutoglu and Ryan (2009), the D-efficiency of a design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ is

$$\mathbf{D_{eff}}(\mathbf{X}) = \left(\frac{\det\left(\mathbf{X}'\ \mathbf{G}^{-1}\mathbf{X}\ \right)}{\det\left(\mathbf{X}_\mathbf{D}'\mathbf{G}^{-1}\mathbf{X}_\mathbf{D}\right)}\right)^{\mathbf{1}/\boldsymbol{p}} \tag{1.3}$$

where $\mathbf{X}_\mathrm{D}$ is a regular D-optimal design.

2. The main result

Let $\mathbf{X}_s \in \mathbf{\Phi}_{(n-s)\times p}\{-1,0,1\}$ be the design matrix of a regular D-optimal chemical balance weighing design with variance matrix of errors $\sigma^2\mathbf{G}$, where for $s = 1,2$, $\mathbf{G}_s = (1-\rho)\mathbf{I}_{n-s} + \rho\mathbf{1}_{n-s}\mathbf{1}'_{n-s}$, i.e. if $\mathbf{X}'_s\mathbf{X}_s = m\mathbf{I}_p$ and $\mathbf{X}'_s\mathbf{1}_{n-s} = \mathbf{0}_p$.

2.1 Supplementation with one measurement, $s = 1$

Let us consider the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X_1} \\ \boldsymbol{x}'_1 \end{bmatrix} \tag{2.1}$$

where $\boldsymbol{x}_1$ is any $p \times 1$ vector of elements equal to $-1, 0$ or 1, $\boldsymbol{x}'_1\boldsymbol{x}_1 = t_1, 1 \leq t_1 \leq p$.

Theorem 2.1. For any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form (2.1) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1),

$$\mathbf{det}(\mathbf{M}) \leq \left(\frac{m}{1-\rho}\right)^{p}\left(1 + \frac{p}{m}\cdot\frac{1+\rho(n-2)}{1+\rho(n-1)}\right). \tag{2.2}$$

Proof. $\mathbf{G}$ is of the form (1.1) and can be written as $\mathbf{G} = \begin{bmatrix} \mathbf{G}_1 & \rho\mathbf{1}_{n-1} \\ \rho\mathbf{1}'_{n-1} & 1 \end{bmatrix}$,

$$\text{and } \mathbf{G}^{-1} = \frac{1}{1-\rho}\begin{bmatrix} \mathbf{I}_{n-1} - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_{n-1}\mathbf{1}'_{n-1} & \frac{-\rho}{1+\rho(n-1)}\mathbf{1}_{n-1} \\ \frac{-\rho}{1+\rho(n-1)}\mathbf{1}'_{n-1} & \frac{1+\rho(n-2)}{1+\rho(n-1)} \end{bmatrix}.$$

Since $\mathbf{X}'_1\mathbf{1}_{n-1} = \mathbf{0}_p$ then $\mathbf{M} = \frac{1}{1-\rho}\left(\mathbf{X}'_1\mathbf{X}_1 + \frac{1+\rho(n-2)}{1+\rho(n-1)}\boldsymbol{x}'_1\boldsymbol{x}_1\right)$ and hence $\det(\mathbf{M}) = \left(\frac{1}{1-\rho}\right)^{p}\det\left(\mathbf{X}'_1\mathbf{X}_1 + \frac{1+\rho(n-2)}{1+\rho(n-1)}\boldsymbol{x}'_1\boldsymbol{x}_1\right)$. By Theorem 18.1.1 in Harville (1997) we have $\det\left(\mathbf{X}'_1\mathbf{X}_1 + \frac{1+\rho(n-2)}{1+\rho(n-1)}\boldsymbol{x}'_1\boldsymbol{x}_1\right) = m^p\frac{1+\rho(n-2)}{1+\rho(n-1)}\left(\frac{1+\rho(n-1)}{1+\rho(n-2)} + \frac{t_1}{m}\right)$. Since the design matrix $\mathbf{X}_1$ is regular D-optimal, $\mathbf{X}'_1\mathbf{X}_1 = m\mathbf{I}_p$ and $\det(\mathbf{M}) = \left(\frac{m}{1-\rho}\right)^{p}\left(1 + \frac{t_1}{m}\cdot\frac{1+\rho(n-2)}{1+\rho(n-1)}\right)$. As we wish to maximize $\det(\mathbf{M})$ under the given matrix $\mathbf{G}$, the function $\det(\mathbf{M})$ is maximal if and only if $t_1 = p$. Hence the theorem.

Definition 2.1. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form (2.1) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is D-optimal if $\det(\mathbf{M}) = \left(\frac{m}{1-\rho}\right)^p \left(1 + \frac{p}{m}\cdot\frac{1+\rho(n-2)}{1+\rho(n-1)}\right)$.

Theorem 2.2. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (2.1) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is D-optimal if

(i) $\mathbf{X}_1'\mathbf{X}_1 = m\mathbf{I}_p$

(ii) $\mathbf{X}_1'\mathbf{1}_{n-1} = \mathbf{0}_p$

(iii) $\boldsymbol{x}_1'\boldsymbol{x}_1 = p$.

Proof. It is clear that $\det(\mathbf{M})$ as given by (2.2) attains its upper bound if conditions (i)–(iii) are fulfilled.

The D-efficiency of a design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (1.3) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is $\mathrm{D}_{\mathrm{eff}}(\mathbf{X}) = \frac{m}{m+1}\sqrt[p]{1 + \frac{p}{m}\cdot\frac{1+\rho(n-2)}{1+\rho(n-1)}}$.

Theorem 2.3. In any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (2.1) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), as the correlation coefficient ρ in (1.1) increases, the efficiency of the design decreases.

Proof. Let us assume that $\rho_1 < \rho_2$ and compare the expressions $\frac{m}{m+1}\sqrt[p]{1 + \frac{p}{m}\cdot\frac{1+\rho_1(n-2)}{1+\rho_1(n-1)}}$ and $\frac{m}{m+1}\sqrt[p]{1 + \frac{p}{m}\cdot\frac{1+\rho_2(n-2)}{1+\rho_2(n-1)}}$. Thus $\frac{1+\rho_1(n-2)}{1+\rho_1(n-1)} - \frac{1+\rho_2(n-2)}{1+\rho_2(n-1)} = \frac{\rho_2-\rho_1}{(1+\rho_1(n-1))(1+\rho_2(n-1))} > 0$. Hence the theorem.

2.2. Supplementation with two measurements, $s = 2$

Let us consider the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X_2} \\ \boldsymbol{x}_1' \\ \boldsymbol{x}_2' \end{bmatrix} \tag{2.3}$$

where $\boldsymbol{x}_1, \boldsymbol{x}_2$ are any $p \times 1$ vectors of elements equal to $-1, 0$ or 1, $\boldsymbol{x}_h'\boldsymbol{x}_h = t_h$, $\boldsymbol{x}_h'\boldsymbol{x}_{h'} = \boldsymbol{x}_{h'}\boldsymbol{x}_h' = u_{hh'}, 1 \leq t_h \leq p, h, h' = 1,2, h \neq h'$.

Theorem 2.4. For any chemical balance weighing design $\mathbf{X} \in \boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$ with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1),

$$\mathbf{det}(\mathbf{M}) \leq \left(\frac{\boldsymbol{m}}{\mathbf{1}-\boldsymbol{\rho}}\right)^{\boldsymbol{p}} \cdot \begin{cases} \left(\mathbf{1}+\frac{\boldsymbol{p}}{\boldsymbol{m}}\right)\left(\mathbf{1}+\frac{\boldsymbol{p}}{\boldsymbol{m}}\cdot\frac{\mathbf{1}+\boldsymbol{\rho}(\boldsymbol{n}-\mathbf{3})}{\mathbf{1}+\boldsymbol{\rho}(\boldsymbol{n}-\mathbf{1})}\right) & \textbf{for even } \boldsymbol{p} \\ \left(\mathbf{1}+\frac{\boldsymbol{p}+\mathbf{1}}{\boldsymbol{m}}\right)\left(\mathbf{1}+\frac{\boldsymbol{p}-\mathbf{1}}{\boldsymbol{m}}\cdot\frac{\mathbf{1}+\boldsymbol{\rho}(\boldsymbol{n}-\mathbf{3})}{\mathbf{1}+\boldsymbol{\rho}(\boldsymbol{n}-\mathbf{1})}\right) & \textbf{for odd } \boldsymbol{p} \end{cases}. \quad (2.4)$$

Proof. $\mathbf{G}$ is of the form (1.1) and can be written as $\mathbf{G} = \begin{bmatrix} \mathbf{G}_2 & \rho\mathbf{1}_{n-2}\mathbf{1}_2' \\ \rho\mathbf{1}_2\mathbf{1}_{n-2}' & (1-\rho)\mathbf{I}_2 + \rho\mathbf{1}_2\mathbf{1}_2' \end{bmatrix}$, and $\mathbf{G}^{-1} = \frac{1}{1-\rho}\begin{bmatrix} \mathbf{I}_{n-2} - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_{n-2}\mathbf{1}_{n-2}' & \frac{-\rho}{1+\rho(n-1)}\mathbf{1}_{n-2}\mathbf{1}_2' \\ \frac{-\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_{n-2}' & \mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2' \end{bmatrix}$. Since $\mathbf{X}_2'\mathbf{1}_{n-2} = \mathbf{0}_p$ then $\mathbf{M} = \frac{1}{1-\rho}\left(\mathbf{X}_2'\mathbf{X}_2 + [\boldsymbol{x}_1 \quad \boldsymbol{x}_2]\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)\begin{bmatrix}\boldsymbol{x}_1' \\ \boldsymbol{x}_2'\end{bmatrix}\right)$ and hence $\det(\mathbf{M}) = \left(\frac{1}{1-\rho}\right)^p \det\left(\mathbf{X}_2'\mathbf{X}_2 + [\boldsymbol{x}_1 \quad \boldsymbol{x}_2]\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)\begin{bmatrix}\boldsymbol{x}_1' \\ \boldsymbol{x}_2'\end{bmatrix}\right)$.

By Theorem 18.1.1 in Harville (1997) we have $\det(\mathbf{M}) = \left(\frac{1}{1-\rho}\right)^p \det(\mathbf{X}_2'\mathbf{X}_2)\det\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)\det\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)^{-1} + \begin{bmatrix}\boldsymbol{x}_1' \\ \boldsymbol{x}_2'\end{bmatrix}(\mathbf{X}_3'\mathbf{X}_3)^{-1}[\boldsymbol{x}_1 \quad \boldsymbol{x}_2]$. Moreover, $\det(\mathbf{X}_2'\mathbf{X}_2)\det\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)\det\left(\mathbf{I}_2 - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_2\mathbf{1}_2'\right)^{-1} + \begin{bmatrix}\boldsymbol{x}_1' \\ \boldsymbol{x}_2'\end{bmatrix}(\mathbf{X}_1'\mathbf{X}_1)^{-1}[\boldsymbol{x}_1 \quad \boldsymbol{x}_2] = \left(\frac{m}{1-\rho}\right)^p \frac{1+\rho(n-3)}{1+\rho(n-1)}\gamma$, where $\gamma = \det\left(\mathbf{I}_2 + \frac{\rho}{1+\rho(n-3)}\mathbf{1}_2\mathbf{1}_2' + \frac{1}{m}\begin{bmatrix}\boldsymbol{x}_1' \\ \boldsymbol{x}_2'\end{bmatrix}[\boldsymbol{x}_1 \quad \boldsymbol{x}_2]\right)$. From the assumption $\boldsymbol{x}_h'\boldsymbol{x}_h = t_h,\ \boldsymbol{x}_h'\boldsymbol{x}_{h'} = u_{hh'},\ h, h' = 1,2,$ $h \neq h'$ it follows that $\gamma = \left(1 + \frac{\rho}{1+\rho(n-3)} + \frac{t_1}{m}\right)\cdot\left(1 + \frac{\rho}{1+\rho(n-3)} + \frac{t_2}{m}\right) - \left(\frac{\rho}{1+\rho(n-3)} + \frac{u_{12}}{m}\right)^2$. The maximum of $\det(\mathbf{M})$ is attained if and only if the maximum of $1 + \frac{\rho}{1+\rho(n-3)} + \frac{t_h}{m}$, $h = 1,2$ and the minimum of $\frac{\rho}{1+\rho(n-3)} + \frac{u_{12}}{m}$ are simultaneously attained. The function $\det(\mathbf{M})$ as a function of $t_h, h = 1,2$, attains its maximal value if and only if $t_h = p, h = 1,2$, and consequently

$$\det(\mathbf{M}) \leq \left(\frac{m}{1-\rho}\right)^{p} \frac{1+\rho(n-3)}{1+\rho(n-1)} \cdot \left[\left(1+\frac{\rho}{1+\rho(n-3)}+\frac{p}{m}\right)^{2} - \left(\frac{\rho}{1+\rho(n-3)}+\frac{u_{12}}{m}\right)^{2}\right].$$

Let us note that u_{12} is the scalar product of two rows of the matrix having elements $-1, 1$, and $u_{12} = 0$ if and only if p is even. In this case

$$\det(\mathbf{M}) \leq \left(\frac{m}{1-\rho}\right)^{p} \left(1+\frac{p}{m}\right)\left(1+\frac{p}{m} \cdot \frac{1+\rho(n-3)}{1+\rho(n-1)}\right).$$

When p is odd, the condition $u_{12} = 0$ is never fulfilled. In this situation, the maximum of $\det(\mathbf{M})$ is attained if and only if u_{12} takes the smallest value -1. Then $\det(\mathbf{M}) \leq \left(\frac{m}{1-\rho}\right)^{p} \left(1+\frac{p+1}{m}\right)\left(1+\frac{p-1}{m} \cdot \frac{1+\rho(n-3)}{1+\rho(n-1)}\right)$. Hence the theorem.

Definition 2.2. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form (2.3) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is D-optimal if

$$\det(\mathbf{M}) = \left(\frac{m}{1-\rho}\right)^{p} \cdot \begin{cases} \left(1+\frac{p}{m}\right)\left(1+\frac{p}{m} \cdot \frac{1+\rho(n-3)}{1+\rho(n-1)}\right) & \textbf{for even } p \\ \left(1+\frac{p+1}{m}\right)\left(1+\frac{p-1}{m} \cdot \frac{1+\rho(n-3)}{1+\rho(n-1)}\right) & \textbf{for odd } p \end{cases}.$$

Theorem 2.5. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (2.3) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), is D-optimal if

(i) $\mathbf{X}_2'\mathbf{X}_2 = m\mathbf{I}_p$

(ii) $\mathbf{X}_2'\mathbf{1}_{n-2} = \mathbf{0}_p$

(iii) $\boldsymbol{x}_h'\boldsymbol{x}_h = p, h = 1,2$

(iv) $u_{12} = \begin{cases} 0 & \text{for even } p \\ -1 & \text{for odd } p \end{cases}$.

Proof. It is easy to see that $\det(\mathbf{M})$ as given by (2.4) attains its upper bound if conditions (i)–(iv) are satisfied.

The D-efficiency of a design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (2.3) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), equals

$$\mathbf{D_{eff}(X)} = \frac{m}{m+2}\begin{cases} \sqrt[p]{\left(1+\frac{p}{m}\right)\left(1+\frac{p}{m}\cdot\frac{1+\rho(n-3)}{1+\rho(n-1)}\right)} & \textbf{for even } p \\ \sqrt[p]{\left(1+\frac{p+1}{m}\right)\left(1+\frac{p-1}{m}\cdot\frac{1+\rho(n-3)}{1+\rho(n-1)}\right)} & \textbf{for odd } p \end{cases}.$$

Theorem 2.6. In any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of the form (2.3) with variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1.1), as the correlation coefficient ρ in (1.1) increases, the efficiency of the design decreases.

The proof is similar to the proof of Theorem 2.3.

3. Examples

Example 3.1. In order to construct the design matrix $\mathbf{X} \in \mathbf{\Phi}_{13\times 6}\{-1,0,1\}$, in accordance with the theory presented above, we consider the matrix $\mathbf{X}_1 \in \mathbf{\Phi}_{12\times 6}\{-1,0,1\}$ in the form

$$\mathbf{X}_1' = \begin{bmatrix} + & - & \mathbf{0} & - & - & \mathbf{0} & - & + & \mathbf{0} & + & + & \mathbf{0} \\ \mathbf{0} & + & - & \mathbf{0} & - & - & \mathbf{0} & - & + & \mathbf{0} & + & + \\ - & \mathbf{0} & + & - & \mathbf{0} & - & + & \mathbf{0} & - & + & \mathbf{0} & + \\ - & - & \mathbf{0} & + & - & \mathbf{0} & + & + & \mathbf{0} & - & + & \mathbf{0} \\ \mathbf{0} & - & - & \mathbf{0} & + & - & \mathbf{0} & + & + & \mathbf{0} & - & + \\ - & \mathbf{0} & - & - & \mathbf{0} & + & + & \mathbf{0} & + & + & \mathbf{0} & - \end{bmatrix},$$

where "+" denotes +1 and "–" denotes –1. Hence, $\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ + \;\; + \;\; + \;\; + \;\; + \;\; + \end{bmatrix}$ is D-optimal in the class $\mathbf{\Phi}_{13\times 6}\{-1,0,1\}$ and $\mathrm{D_{eff}}(\mathbf{X}) = \frac{8}{9}\sqrt[6]{1+\frac{6}{8}\cdot\frac{1+11\rho}{1+12\rho}}$. In particular cases, when $\rho = 0.1$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.97273$, and when $\rho = 0.2$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.971164$.

Example 3.2. In order to construct the design matrix $\mathbf{X} \in \mathbf{\Phi}_{6\times 4}\{-1,0,1\}$, in accordance with the theory presented above, we consider the matrix $\mathbf{X}_1 \in \mathbf{\Phi}_{4\times 4}\{-1,0,1\}$ in the form $\mathbf{X}_1' = \begin{bmatrix} + & + & + & - \\ + & + & - & + \\ + & - & + & + \\ - & + & + & + \end{bmatrix}$. Therefore, $\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ + \;\; + \;\; + \;\; + \\ + \;\; + \;\; - \;\; - \end{bmatrix}$ is D-optimal in the class $\mathbf{\Phi}_{6\times 4}\{-1,0,1\}$ and

$\mathrm{D_{eff}}(\mathbf{X}) = \frac{2}{3}\sqrt[4]{1+\frac{1+3\rho}{1+5\rho}}$. In particular cases, when $\rho = 0.1$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.926687$, and when $\rho = 0.2$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.891654$.

Example 3.3. In order to construct the design matrix $\mathbf{X} \in \mathbf{\Phi}_{30\times 7}\{-1,0,1\}$, in accordance with the theory presented above, we consider the matrix $\mathbf{X}_1 \in \mathbf{\Phi}_{28\times 7}\{-1,0,1\}$ in the form $\mathbf{X}_1' = [\mathbf{X}_{11} \quad \mathbf{X}_{12}]$, where

$$\mathbf{X_{11}} = \begin{bmatrix} + & - & - & - & + & - & + \\ + & + & - & - & - & + & - \\ - & + & + & - & - & - & + \\ + & - & + & + & - & - & - \\ - & + & - & + & + & - & - \\ - & - & + & - & + & + & - \\ - & - & - & + & - & + & + \end{bmatrix}$$

$$\mathbf{X_{12}} = \begin{bmatrix} - & - & - & - & - & - & - \\ + & + & + & + & - & - & - \\ - & - & - & - & + & + & + \\ + & - & - & - & + & - & - \\ - & + & - & - & - & + & - \\ - & - & + & - & - & - & + \\ - & - & - & + & - & - & - \end{bmatrix}$$

Therefore, $\mathbf{X} = \begin{bmatrix} & & & \mathbf{X_1} & & & \\ + & + & - & + & + & - & + \\ + & - & + & + & - & + & + \end{bmatrix}$ is D-optimal in the class $\mathbf{\Phi}_{30\times 7}\{-1,0,1\}$ and $\mathrm{D_{eff}}(\mathbf{X}) = \frac{14}{15}\sqrt[7]{\frac{29}{15}\left(1+\frac{3}{14}\cdot\frac{1+27\rho}{1+29\rho}\right)}$. In particular cases, when $\rho = 0.1$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.993369$, and when $\rho = 0.2$, $\mathrm{D_{eff}}(\mathbf{X}) = 0.993178$.

4. Discussion

Bounds of the determinant of the information matrix for a chemical balance weighing design have been given. These bounds are presented under the assumption that the measurement errors are equally correlated and they have the same variances. However, it is not possible to determine a D-optimal chemical balance weighing design in any class of matrices having elements $-1,0,1$. Hence the above proposal for the construction of the aforementioned design. Moreover,

further possibilities of constructing these designs based on the known matrices of block designs should be considered. The theoretical results were illustrated by examples of construction for three special cases. It is worth noting, among the various applications of weighing systems, the following studies related to agricultural experimentation: Ceranka and Katulska (1987, 1989) and Katulska (1984). Graczyk (2013) describes the possibility of using the weighing design matrix as an experiment plan in plant protection studies, and Graczyk (2014) describes an experiment plan for comparing the impact of NPK and various types of organic matter used under the fore crop on the health condition of the stem base of the successor plant, namely spring barley. Further research may be directed towards the determination of optimal designs in classes in which it has not been possible to do so with the use of known construction methods.

REFERENCES

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. (2014): The problem of D-optimality in some experimental designs. International Journal of Mathematics and Computer Application Research 4: 11–18.

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

Ceranka B., Graczyk M. (2015): D-optimal designs with negative correlated errors based on ternary designs: construction. Colloquium Biometricum 145: 35–45.

Ceranka B., Graczyk M. (2016): New construction of D-optimal weighing designs with non-negative correlations of errors. Colloquium Biometricum 46: 31–46.

Ceranka B., Graczyk M. (2018): Highly D-efficient weighing designs for an even number of objects. Revstat Statistical Journal 16(4): 475–486.

Ceranka, B., Katulska, K. (1987): Zastosowanie teorii sprężynowych układów wagowych do analizy doświadczeń z mieszankami. *Listy Biometryczne* XXIV: 17–26.

Ceranka B., Katulska K. (1989): Application of the biased spring balance weighing theory to estimation of differences of line effects for legume content. Biometrical Journal 31: 103–110.

Graczyk M. (2013): Some applications on weighing designs. Biometrical Letters 50: 15–26.

Graczyk M. (2014): Relations between randomized block designs and weighing designs in examples. Colloquium Biometricum 44: 97–107.

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

Katulska K. (1984): Zastosowanie teorii układów wagowych do badania upraw paszowych i w geodezji. Czternaste Colloquium Metodologiczne z Agro-Biometrii, PAN: 195–208.