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Estimation of Unknown Object Measures in a Chemical Weighing Design with Correlated Errors

Abstract:

In this paper, some problems that concern the determining of unknown measurements of objects in the model of a chemical balance weighing design are presented. These designs are tested under the assumption that measurement errors are correlated and have the same variances. The relations between the parameters of a weighing design are considered from the point of view of the D-optimality criterion. We give some conditions determining the dependencies between the parameters of such designs and construction examples.

Keywords:

chemical balance weighing design, D-efficient design, D-optimal design

JEL:

C02, C18, C90

1. Introduction

In our study, we consider the linear model $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where \mathbf{y} is an $n \times 1$ random vector of observed measurements, $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$, having elements equal to $-1, 0$ or 1 , $i = 1, 2, \dots, n$, $j = 1, 2, \dots, p$. Here, \mathbf{w} is a $p \times 1$ vector representing unknown ob-

jects measures, \mathbf{e} is an $n \times 1$ vector of random errors. Moreover, we assume that there are no systematic errors, the errors are uncorrelated, and they have different variances, i.e., $E(\mathbf{e}) = \mathbf{0}_n$, $\text{Var}(\mathbf{e}) = \sigma^2 \mathbf{G}$, where $\sigma > 0$ is a known parameter, $\mathbf{G} = (1 - \rho)\mathbf{I}_n + \rho \mathbf{1}_n \mathbf{1}_n'$ is the $n \times n$ positive definite matrix of known elements, $0 < \rho < 1$.

The applications of chemical balance weighing designs are unlimited and involve economic surveys, see Banerjee (1975), Graczyk (2013), as well as bioengineering, see Gawande and Patkar (1999). Selected problems considered in the literature on weighing designs are connected with optimality criteria, see Koukouvinos (1996), and with new construction methods, see Gail and Kiefer (1982), Ceranka and Graczyk (2010; 2012), as well as Katulska and Smaga (2010).

To get the estimator of the vector of unknown measurements of objects \mathbf{w} , you need to use the normal equation $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{G}^{-1}\mathbf{y}$. On the understanding that \mathbf{G} is a known positive definite matrix, $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}$ is nonsingular if and only if \mathbf{X} is of full column rank. In that case, the generalised least squares estimator of \mathbf{w} is given by $\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{G}^{-1}\mathbf{y}$ and $\text{Var}(\hat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}$.

2. The main result

Among the various possible optimality criteria considered in the literature, we chose criterion D, which minimises the product of the variances of the estimators. The concept of D-optimal design was presented in Raghavarao (1971), Banerjee (1975), Shah and Sinha (1989), Ceranka and Graczyk (2019). Let us recall the definitions of D-optimal design.

Definition 2.1. The design \mathbf{X} is regular D-optimal in the class $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ if $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1} = \min \left\{ \det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1} : \mathbf{X} \in \Phi_{n \times p}(-1, 0, 1) \right\}$.

Not for every possible combination of number of objects and number of measurements are we able to determine the optimal design. In such a situation, a highly D-efficient design is considered Bulutoglu and Ryan (2009).

Definition 2.2. The design \mathbf{X} is highly D-efficient in the class $\Phi_{n \times p}(-1, 0, 1)$ for the given variance matrix of errors $\sigma^2 \mathbf{G}$, if $D_{\text{eff}}(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})}{\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})} \right]^{1/p} \geq 0.95$, where \mathbf{Y} is the matrix of D-optimal spring balance weighing design for the same variance matrix of errors $\sigma^2 \mathbf{G}$.

The purpose of this paper is to present new results on construction methods and to determine the conditions for the existence of correlated with D-optimal and highly D-efficient spring balance designs under the assumption that random errors are correlated and have the same variances. We present such results from the point of view of the special form of the variance matrix of errors.

Let $\mathbf{X}_1 \in \Phi_{(n-1) \times p}(-1, 0, 1)$ be the design matrix of a regular D-optimal chemical balance weighing design with the variance matrix of errors $\sigma^2 \mathbf{G}_1 = \sigma^2 \left((1-\rho) \mathbf{I}_{n-1} + \rho \mathbf{1}_{n-1} \mathbf{1}_{n-1}' \right)$, $0 < \rho < 1$, i.e. $\mathbf{X}_1' \mathbf{X}_1 = m \mathbf{I}_p$ and $\mathbf{X}_1' \mathbf{1}_{n-1} = \mathbf{0}_p$.

2.1. Admixing one measurement

Now, let us consider the design matrix $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form:

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1' & \mathbf{x}_1' \end{bmatrix}, \quad (2.1)$$

with the variance matrix of errors $\sigma^2 \mathbf{G}$ given by the formula:

$$\mathbf{G} = \begin{bmatrix} \mathbf{G}_1 & \mathbf{0}_{n-1} \\ \mathbf{0}_{n-1}' & 1 \end{bmatrix}, \quad (2.2)$$

where \mathbf{x}_1 is any vector of elements $-1, 0, 1$, $\mathbf{x}_1' \mathbf{x}_1 = t_1$, $1 \leq t_1 \leq p$.

Theorem 2.1. In any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form (2.1)

with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.2),

$$\det(\mathbf{X}' \mathbf{G}^{-1} \mathbf{X}) \leq \left(\frac{m}{1-\rho} \right)^p \left(1 + \frac{(1-\rho)p}{m} \right). \quad (2.3)$$

Proof. For \mathbf{G} which is of the form (2.2), we have $\mathbf{G}^{-1} = \begin{bmatrix} \mathbf{I}_{n-1} - \frac{\rho}{1+\rho(n-2)} \mathbf{1}_{n-1} \mathbf{1}_{n-1}' & \mathbf{0}_{n-1} \\ \mathbf{0}_{n-1}' & 1-\rho \end{bmatrix}$.

Since $\mathbf{X}_1' \mathbf{1}_{n-1} = \mathbf{0}_p$, then $\mathbf{X}' \mathbf{G}^{-1} \mathbf{X} = \frac{\rho}{1-\rho} [\mathbf{X}_1' \mathbf{X}_1 + (1-\rho) \mathbf{x}_1 \mathbf{x}_1']$ and hence

$\det(\mathbf{X}' \mathbf{G}^{-1} \mathbf{X}) = \frac{\rho}{1-\rho} \det(\mathbf{X}_1' \mathbf{X}_1 + (1-\rho) \mathbf{x}_1 \mathbf{x}_1')$. According to the Theorem 18.1.1 in Harville (1997),

we get $\det(\mathbf{X}_1' \mathbf{X}_1 + (1-\rho) \mathbf{x}_1 \mathbf{x}_1') = m^p \left(1 + \frac{(1-\rho)t_1}{m} \right)$. Our goal is to choose the matrix

$\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ such that the determinant $\det(\mathbf{X}' \mathbf{G}^{-1} \mathbf{X})$ is maximal. We know that $\det(\mathbf{X}' \mathbf{G}^{-1} \mathbf{X})$ as the function of variable t_1 attains the maximal value if and only if $t_1 = p$. Hence the Theorem.

Definition 2.3. Any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form (2.1) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.2), is D-optimal if

$$\det(\mathbf{X}' \mathbf{G}^{-1} \mathbf{X}) = \left(\frac{m}{1-\rho} \right)^p \left(1 + \frac{(1-\rho)p}{m} \right).$$

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

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

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

$$\mathbf{x}'_1 \mathbf{x}_1 = p.$$

Proof. It is easy to observe that if conditions (i)-(iii) are satisfied, then $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$ given in (2.3) is maximal.

$$\text{According to the Definition 2.2, } D_{\text{eff}}(\mathbf{x}) = \frac{m}{m+1} \sqrt[p]{1 + \frac{(1-\rho)p}{m}}.$$

Theorem 2.3. For any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}\{-1, 0, 1\}$ of the form (2.1) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.2), $D_{\text{eff}}(\mathbf{X})$ is a decreasing

$$\text{function of the variable } \rho \text{ and } D_{\text{eff}}(\mathbf{X}) \in \left(\frac{m^{\frac{p-1}{p}} (m+p)^{\frac{1}{p}}}{m+1}, \frac{m}{m+1} \right).$$

Proof. We consider $\frac{m}{m+1} \sqrt[p]{1 + \frac{(1-\rho_1)p}{m}} > \frac{m}{m+1} \sqrt[p]{1 + \frac{(1-\rho_2)p}{m}}$. Hence $1 + \frac{(1-\rho_2)p}{m} > 1 + \frac{(1-\rho_1)p}{m}$ and $\rho_1 < \rho_2$. Moreover, $\lim_{\rho \rightarrow 0} (D_{\text{eff}}(\mathbf{x})) = \frac{m^{\frac{p-1}{p}} (m+p)^{\frac{1}{p}}}{m+1}$,

$\lim_{\rho \rightarrow 1} (D_{\text{eff}}(\mathbf{x})) = \frac{m}{m+1}$. Hence the Theorem.

2.2. Admixing two measurements

Let $\mathbf{X}_2 \in \Phi_{(n-2) \times p}(-1, 0, 1)$ be the design matrix of a regular D-optimal chemical balance weighing design with the variance matrix of errors $\sigma^2 \mathbf{G}_2 = \sigma^2 ((1-\rho) \mathbf{I}_{n-2} + \rho \mathbf{1}_{n-2} \mathbf{1}'_{n-2})$, $0 < \rho < 1$, i.e. $\mathbf{X}'_2 \mathbf{X}_2 = m \mathbf{I}_p$ and $\mathbf{X}'_2 \mathbf{1}_{n-2} = \mathbf{0}_p$, given by the form:

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}'_2 & \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}', \quad (2.4)$$

with the variance matrix of errors $\sigma^2 \mathbf{G}$ given by the formula:

$$\mathbf{G} = \begin{bmatrix} \mathbf{G}_2 & \mathbf{0}_{n-2} \\ \mathbf{0}'_{n-2} & \mathbf{I}_2 \end{bmatrix}, \quad (2.5)$$

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

Theorem 2.4. In any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form (2.4) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.5),

(i) If p is even, then:

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leq \left(\frac{m}{1-\rho}\right)^p \left(1 + \frac{(1-\rho)p}{m}\right)^2. \quad (2.6)$$

(ii) If p is odd, then:

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leq \left(\frac{m}{1-\rho}\right)^p \left(1 + \frac{(1-\rho)(p+1)}{m}\right) \left(1 + \frac{(1-\rho)(p-1)}{m}\right). \quad (2.7)$$

Proof. For \mathbf{G} which is of the form (2.5), we have $\mathbf{G}^{-1} = \begin{bmatrix} \mathbf{I}_{n-2} - \frac{\rho}{1+\rho(n-3)} \mathbf{1}_{n-2} \mathbf{1}_{n-2}' & \mathbf{0}_{n-2} \mathbf{0}_2' \\ \mathbf{0}_2 \mathbf{0}_{n-2}' & (1-\rho) \mathbf{I}_2 \end{bmatrix}$.

Since $\mathbf{X}_2' \mathbf{1}_{n-2} = \mathbf{0}_p$, then $\mathbf{x}' \mathbf{G}^{-1} \mathbf{x} = \frac{\rho}{1-\rho} [\mathbf{X}_2' \mathbf{X}_2 + (1-\rho)(\mathbf{x}_1 \mathbf{x}_1' + \mathbf{x}_2 \mathbf{x}_2')] \quad \text{and} \quad \text{hence}$

$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) = \left(\frac{\rho}{1-\rho}\right)^p \det(\mathbf{X}_2' \mathbf{X}_2 + (1-\rho)(\mathbf{x}_1 \mathbf{x}_1' + \mathbf{x}_2 \mathbf{x}_2'))$. Considering the fact that \mathbf{X}_2 is the ma-

trix of the regular D-optimal design and based on Theorem 18.1.1 in Harville (1997), we obtain the following:

$$\det\left(\mathbf{X}_2' \mathbf{X}_2 + [\mathbf{x}_1 \quad \mathbf{x}_2](1-\rho) \mathbf{I}_2 \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \end{bmatrix}\right) = \det(\mathbf{X}_2' \mathbf{X}_2) \det((1-\rho) \mathbf{I}_2) \cdot \det((1-\rho) \mathbf{I}_2)^{-1} +$$

$\begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \end{bmatrix} (\mathbf{X}_2' \mathbf{X}_2)^{-1} [\mathbf{x}_1 \quad \mathbf{x}_2] = m^p (1-\rho)^2 \cdot \gamma$, where $\gamma = \det\left(\frac{1}{1-\rho} \mathbf{I}_2 + \frac{1}{m} \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \end{bmatrix} [\mathbf{x}_1 \quad \mathbf{x}_2]\right)$. From the as-

sumptions $\mathbf{x}_h' \mathbf{x}_h = t_h$, $1 \leq t_h \leq p$, $\mathbf{x}_h' \mathbf{x}_{h'} = u_{hh'}$, $h, h' = 1, 2, h \neq h'$, it follows that

$\gamma = \left(\frac{1}{1-\rho} + \frac{t_1}{m}\right) \left(\frac{1}{1-\rho} + \frac{t_2}{m}\right) - \left(\frac{u_{12}}{m}\right)^2$. The maximal value of $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$ is attained if and only

if the expression $\frac{1}{1-\rho} + \frac{t_h}{m}$, $h=1,2$, attains the maximal value and simultaneously the expres-

sion $\left(\frac{u_{12}}{m}\right)^2$ attains the minimal value. We know that $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$, as a function of t_h , $h=1,2$,

and attains maximum if and only if $t_h = p$, $h=1,2$, and consequently

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leq \left(\frac{m}{1-\rho}\right)^p (1-\rho)^2 \left(\left(\frac{1}{1-\rho} + \frac{p}{m}\right)^2 - \left(\frac{u_{12}}{m}\right)^2\right).$$

Let us note that u_{12} is the scalar product of two rows of the matrix having elements $-1, 0, 1$ and $u_{12} = 0$ if and only if p is even. In this case, $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leq \left(\frac{m}{1-\rho}\right)^p \left(1 + \frac{(1-\rho)p}{m}\right)^2$. When p is odd, the condition $u_{12} = 0$ is never fulfilled. So, for odd numbers of objects, the maximum of $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$ is attained if and only if $u_{12} = \pm 1$. Then $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leq \left(\frac{m}{1-\rho}\right)^p \left(1 + \frac{(1-\rho)(p+1)}{m}\right) \left(1 + \frac{(1-\rho)(p-1)}{m}\right)$. Hence the Theorem.

Definition 2.4. Any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form (2.4) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.5), is D-optimal if:

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) = \left(\frac{m}{1-\rho}\right)^p \cdot \begin{cases} \left(1 + \frac{(1-\rho)p}{m}\right)^2 & \text{for even } p \\ \left(1 + \frac{(1-\rho)(p+1)}{m}\right) \left(1 + \frac{(1-\rho)(p-1)}{m}\right) & \text{for odd } p \end{cases}.$$

Theorem 2.5. Any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in the form (2.4) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.5), 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) $\mathbf{x}'_h \mathbf{x}_h = p, h = 1, 2$
- (iv) $u_{12} = \begin{cases} 0 & \text{for even } p \\ \pm 1 & \text{for odd } p \end{cases}.$

Proof. It is easy to observe that if conditions (i)–(iv) are satisfied, then $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$ given in (2.6) and (2.7) is maximal.

According to the Definition 2.2:

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

Theorem 2.6. For any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}\{-1, 0, 1\}$ of the form (2.4) with the variance matrix of errors $\sigma^2 \mathbf{G}$, where \mathbf{G} is of the form (2.5), $D_{\text{eff}}(\mathbf{X})$ is a decreasing

function of the variable ρ and $D_{\text{eff}}(\mathbf{X}) \in \begin{cases} \left(\frac{m^{\frac{p-2}{p}} (m+p)^{\frac{2}{p}}}{m+2}, \frac{m}{m+2} \right) & \text{for even } p \\ \left(\frac{m^{\frac{p-2}{p}} ((m+p)^2 - 1)^{\frac{1}{p}}}{m+2}, \frac{m}{m+2} \right) & \text{for odd } p \end{cases}.$

Proof. The proof is analogous to that given in Theorem 2.3.

3. Examples

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

$$\mathbf{X}'_1 = \begin{bmatrix} + & - & 0 & - & - & 0 & - & + & 0 & + & + & 0 \\ 0 & + & - & 0 & - & - & 0 & - & + & 0 & + & + \\ - & 0 & + & - & 0 & - & + & 0 & - & + & 0 & + \\ - & - & 0 & + & - & 0 & + & + & 0 & - & + & 0 \\ 0 & - & - & 0 & + & - & 0 & + & + & 0 & - & + \\ - & 0 & - & - & 0 & + & + & 0 & + & + & 0 & - \end{bmatrix}, \text{ where '+' denotes '+1' and '-' denotes '-1.'}$$

Hence, $\mathbf{X} = \begin{bmatrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix} \begin{matrix} \mathbf{X}_1 \\ + \\ + \\ + \\ + \\ + \\ + \end{matrix}$ is D-optimal in the class $\Phi_{13 \times 6} \{-1, 0, 1\}$ and

$$D_{\text{eff}}(\mathbf{X}) = \frac{8}{9} \sqrt[6]{1 + \frac{6}{8} \frac{1+11\rho}{1+12\rho}}.$$

Example 3.2. In order to construct the design matrix $\mathbf{X} \in \Phi_{6 \times 4} \{-1, 0, 1\}$, according to the pre-

sented theory, we consider matrix $\mathbf{X}_1 \in \Phi_{4 \times 4} \{-1, 0, 1\}$ in the form $\mathbf{X}'_2 = \begin{bmatrix} + & + & + & - \\ + & + & - & + \\ + & - & + & + \\ - & + & + & + \end{bmatrix}$. Therefore,

$$\mathbf{X} = \begin{bmatrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix} \begin{matrix} \mathbf{X}_2 \\ + \\ + \\ + \\ + \\ + \end{matrix} \text{ is D-optimal in the class } \Phi_{6 \times 4} \{-1, 0, 1\} \text{ and } D_{\text{eff}}(\mathbf{X}) = \frac{2}{3} \sqrt[4]{1 + \frac{1+3\rho}{1+5\rho}}.$$

Example 3.3. In order to construct the design matrix $\mathbf{X} \in \Phi_{30 \times 7} \{-1, 0, 1\}$, according to the presented theory, we consider matrix $\mathbf{X}_2 \in \Phi_{28 \times 7} \{-1, 0, 1\}$ in the form $\mathbf{X}'_2 = [\mathbf{X}_{21} \quad \mathbf{X}_{22}]$, where:

$$\mathbf{X}_{21} = \begin{bmatrix} + & - & - & - & + & - & + & + & + & + & + & + & + & - \\ + & + & - & - & - & + & - & + & - & - & - & - & - & + \\ - & + & + & - & - & - & + & - & + & - & - & - & - & + \\ + & - & + & + & - & - & - & - & - & + & - & - & - & - \\ - & + & - & + & + & - & - & - & - & - & + & - & - & - \\ - & - & + & - & + & + & - & - & - & - & - & + & - & - \\ - & - & - & + & - & + & + & - & - & - & - & - & + & - \end{bmatrix},$$

$$\mathbf{X}_{22} = \begin{bmatrix} - & - & - & - & - & - & - & - & - & - & - & - & - & - \\ + & + & + & + & - & - & - & - & - & - & - & - & - & - \\ - & - & - & - & + & + & + & + & - & - & - & - & - & - \\ + & - & - & - & + & - & - & - & + & + & + & - & - & - \\ - & + & - & - & - & + & - & - & + & - & - & + & + & - \\ - & - & + & - & - & - & + & - & - & + & - & + & - & + \\ - & - & - & + & - & - & - & + & - & - & + & - & + & + \end{bmatrix}.$$

Therefore, $\mathbf{X} = \begin{bmatrix} & & & \mathbf{X}_2 & & \\ + & + & - & + & + & - & + \\ + & - & + & + & - & + & + \end{bmatrix}$ is D-optimal in the class $\Phi_{30 \times 7} \{-1, 0, 1\}$ and

$$D_{\text{eff}}(\mathbf{X}) = \frac{14}{15} \sqrt[7]{\frac{29}{15} \left(1 + \frac{3}{14} \cdot \frac{1+27\rho}{1+29\rho} \right)}.$$

D-efficiency for designs determined in examples

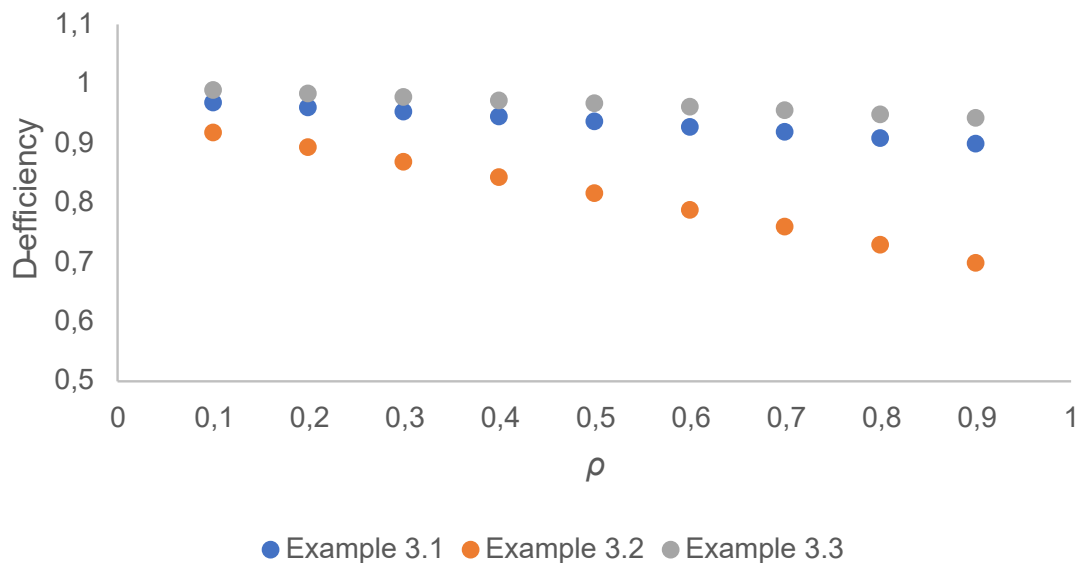


Figure 1. Comparison of the D-efficiency for designs $\mathbf{X} \in \Phi_{13 \times 6} \{-1, 0, 1\}$ (Example 3.1), $\mathbf{X} \in \Phi_{6 \times 4} \{-1, 0, 1\}$ (Example 3.2) and $\mathbf{X} \in \Phi_{30 \times 7} \{-1, 0, 1\}$, (Example 3.3), determined for $\rho \in \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$.

Source: own calculations

4. Conclusions

In the literature, many works that give conditions which determine the existence of D-optimal systems are presented. However, not for every pair: the number of objects and the number of measurements, can we determine a design that meets the criterion of D-optimality. For this reason, in the presented considerations, we dealt with the determination of new methods of construction of the matrix of the system. Their purpose is to make it possible to determine the matrix of a D-optimal design in classes that are not yet known in the literature. This goal was achieved by adding to the D-optimal matrix determined in the class for $n - k$ measurements and p objects $k, k = 1, 2$, measurements. Consequently, the key result obtained in the work is to give an assessment of the determinant of the information matrix and to give conditions determining the D-optimal design.

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Estymacja nieznanymi miar obiektów w chemicznym układzie wagowym ze skorelowanymi błędami

Streszczenie:



W artykule przedstawiono problemy dotyczące wyznaczenia nieznanymi miar obiektów w modelu chemicznego układu wagowego. Układy te są analizowane przy założeniu, że błędy pomiarów są skorelowane i mają jednakowe wariancje. Zależności pomiędzy parametrami układów są analizowane z punktu widzenia kryterium D-optimalności. Podane zostały warunki określające parametry układów oraz przykładowe konstrukcje.

Słowa kluczowe:

chemiczny układ wagowy, układ D-efektywny, układ D-optimalny

JEL:

C02, C18, C90

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