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ABOUT SOME PROPERTIES AND CONSTRUCTIONS OF EXPERIMENTAL DESIGNS

Abstract. In this paper, we consider the problems related to the determining plan of the experiment performed according to the model of the chemical balance weighing design under additional assumption that the experimental errors are equally negatively correlated. This problem is studied from the point of view of D-optimality of such a design. We give new a construction method of D-optimal chemical balance weighing design and the list of possible experimental plans.

Keywords: balanced incomplete block design, chemical balance weighing design, D-optimality, ternary balanced block design.

JEL: C10, C90

1. INTRODUCTION

Let us consider the experiment whose results are represented as a linear combination of unknown measurements of p objects with factors of this combination equal to -1, 0 or 1. Therefore, $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where $\mathbf{y}$ is an $n \times 1$ random vector of observed weights, $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$, $\mathbf{\Phi}_{n\times p}(-1,0,1)$ is the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$, $i = 1,2,...,n$, $j = 1,2,..., p$, of known elements equal to -1, 1 or 0. Furthermore, $\mathbf{w}$ is a $p \times 1$ vector of unknown measurements of objects and $\mathbf{e}$ is an $n \times 1$ vector of random errors. Let us assume that there are no systematic errors, i.e. $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and the errors are equally, negatively correlated with equal variances, i.e. $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{0}_n$ is vector of zeros, $\sigma > 0$ is known parameter, $\mathbf{G}$ is the $n \times n$ symmetric positive definite diagonal matrix of known elements given in the form

$$\mathbf{G} = g\left[(1-\rho)\mathbf{I}_n + \rho\mathbf{1}_n\mathbf{1}_n^{'}\right], \quad g > 0, \frac{-1}{n-1} < \rho < 0, \tag{1}$$

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$\mathbf{I}_n$ denotes identity matrix of rank n and $\mathbf{1}_n$ denotes $n \times 1$ vector with 1 element everywhere.

The inverse of matrix $\mathbf{G}$ is given as $\mathbf{G}^{-1} = (g(1-\rho))^{-1}\left[\mathbf{I}_n - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_n\mathbf{1}_n^{'}\right]$. For the estimation of unknown measurements of objects $\mathbf{w}$ we use the normal equations $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X} = \mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{y}$. Any chemical balance weighing design is nonsingular, depending on whether $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is nonsingular. $\mathbf{G}$ is a known positive definite matrix that is why $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is nonsingular if and only if $\mathbf{X}$ is of full column rank. By the time $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is nonsingular the generalized least squares estimator of $\mathbf{w}$ is given by $\hat{\mathbf{w}} = \left(\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{y}$ and $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\left(\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\right)^{-1}$. Matrix $\mathbf{M} = \mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is called the information matrix of the design $\mathbf{X}$.

Any possible optimality criterion of experimental designs is functional of the information matrix. For each form of the variance matrix of errors $\mathbf{G}$ and for each optimality criterion, the conditions determining optimal design and construction methods are studied separately. In the present paper we study, among many optimality criteria, the properties of D-optimal designs. The design $\mathbf{X}_d$ is D-optimal in the class of the design matrices $\mathbf{\Psi} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$, if $\det\left(\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\right) = \max\{\det\mathbf{M} : \mathbf{X} \in \mathbf{\Psi}\}$. It is known, $\det\mathbf{M}$ is maximal if and only if $\det\mathbf{M}^{-1}$ is minimal. The problems related to the determining D-optimal designs were considered in the literature (Raghavarao 1971, Banerjee 1975, Shah and Sinha 1989, Jacroux et al. 1983). Furthermore, D-optimal weighing designs determined in the class $\mathbf{\Xi}_{n\times p}(-1,1)$ were presented in many papers (Masaro and Wong 2008, Katulska and Smaga 2013), where $\mathbf{\Xi}_{n\times p}(-1,1)$ is the set of all $n \times p$ matrices $\mathbf{X} = (x_{ij})$ with elements equal to -1, or 1 only.

In the paper, we present new results related to the D-optimal chemical balance weighing designs assuming that the random errors are equally negative correlated and with the same variances. We construct the design matrix of D-optimal design based on the incidence matrices of the balanced incomplete block designs and the ternary balanced block designs. We give the lower bound for the determinant of the inverse of the information matrix and the list of the parameters of D-optimal experimental plans.

2. D-OPTIMAL DESIGNS

In order to determine the lower bound of $\det\left(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}\right)^{-1} = \min\{\det\mathbf{M} : \mathbf{X} \in \mathbf{\Psi}\}$ from among matrices in the class $\mathbf{\Phi}_{n\times p}(-1,0,1)$, let us consider $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_p] \in \mathbf{\Phi}_{n\times p}(-1,0,1)$. Based on the results given in Rao 1973: Section 1c.1 (ii) (b) we get.

Lemma 1. For diagonal elements of the inverse of information matrix, the inequality $M_{jj}^{-1} = \left(\mathbf{x}_j'\mathbf{G}^{-1}\mathbf{x}_j\right)^{-1} \geq g(1-\rho)\left(\mathbf{x}_j'\mathbf{x}_j - \frac{\mathbf{x}_j'\mathbf{1}_n\mathbf{1}_n'\mathbf{x}_j\rho}{1+\rho(n-1)}\right)^{-1}$ holds.

Next, we prove the inequality which gives the lower bound for determinant $\mathbf{M}^{-1}$.

Theorem 1. If $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ and $\mathbf{G}$ is given in (1) then

$$\det\mathbf{M}^{-1} \geq \left(g(1-\rho)\left(m - \frac{\rho(m-2u)^2}{1+\rho(n-1)}\right)^{-1}\right)^p, \tag{2}$$

where $m = \max\{m_1, m_2, ..., m_p\}$, m_j represents the number of elements equal to -1 and 1 in j^{th} column of $\mathbf{X}$, $u = \min\{u_1, u_2, ..., u_p\}$, u_j represents the number of elements equal to -1 in j^{th} column of $\mathbf{X}$, $j = 1,2,..., p$.

Proof. Our proof starts with the observation that by the Hadamard's inequality the determinant of $\mathbf{M}^{-1}$ is greater or equal than the product of diagonal elements of this matrix, i.e. $\det\left(\mathbf{M}^{-1}\right) \geq \prod_{j=1}^{p} M_{jj}^{-1} = \prod_{j=1}^{p}\left(\mathbf{x}_j'\mathbf{G}^{-1}\mathbf{x}_j\right)^{-1}$. By Lemma 1 we conclude that (2) holds, since elements of $\mathbf{x}_j$ are equal to -1, 0, 1 only. Thus, we get the thesis.

Definition 1. Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given in (1), is said to be regular D-optimal if it satisfies the equality in (2), that is $\det\mathbf{M}^{-1} = \left(g(1-\rho)\left(m - \frac{\rho(m-2u)^2}{1+\rho(n-1)}\right)^{-1}\right)^p$.

Let us note, the regular D-optimal design is D-optimal, whereas the inverse sentence is not true. Moreover, for the case $\frac{-1}{n-1} < \rho < 0$, if $\rho \to \frac{-1}{n-1}$ then $\det \mathbf{M}^{-1} \to \infty$.

The conditions determining the regular D-optimal design are given in the literature (Ceranka and Graczyk 2014 a).

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

(i) $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p - \frac{\rho(m-2u)^2}{1+\rho(n-1)}\left(\mathbf{I}_p - \mathbf{1}_p\mathbf{1}_p'\right)$ and

(ii) $\mathbf{X}'\mathbf{1}_n = \mathbf{z}_p$,

where $\mathbf{z}_p$ is $p \times 1$ vector, for which the j^{th} element is equal to $m-2u$ or $-(m-2u)$, $j = 1,2,...,p$.

3. CONSTRUCTION OF REGULAR D-OPTIMAL DESIGNS

Some methods of constructions regular D-optimal designs were given by Masaro and Wong (2008) and Katulska and Smaga (2013) for the case $\mathbf{X} \in \mathbf{\Xi}_{n\times p}(-1,1)$. Furthermore, in the class $\mathbf{\Phi}_{n\times p}(-1,0,1)$ for non-negative correlated measurement errors, the construction based on the incidence matrices of the balanced bipartite weighing designs and the ternary balanced block designs were given in Ceranka and Graczyk (2014b, c). The construction based on the incidence matrices of the balanced bipartite weighing designs, for negative correlated measurement errors was introduced in Ceranka and Graczyk (2014d). Here, we broaden the list of classes $\mathbf{\Phi}_{n\times p}(-1,0,1)$ in which regular D-optimal chemical balance weighing design exists.

Therefore, in this section, we present a new construction of regular D-optimal chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ based on the incidence matrices of the balanced incomplete block design and the ternary balanced block design.

Let $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ be the design matrix of the chemical balance weighing design in the form

$$\mathbf{X}=\begin{bmatrix} 2\mathbf{N}_1^{'}-\mathbf{1}_{b_1}\mathbf{1}_v^{'} \\ \mathbf{N}_2^{'}-\mathbf{1}_{b_2}\mathbf{1}_v^{'} \end{bmatrix}, \tag{3}$$

where $\mathbf{N}_1$ is the incidence matrix of the balanced incomplete block design with the parameters v, b_1, r_1, k_1, λ_1 (Raghavarao and Padgett, 2005) and $\mathbf{N}_2$ is the incidence matrix of the ternary balanced block design with the parameters v, b_2, r_2, k_2, λ_2, ρ_{12}, ρ_{22} (see Billington, 1984). For the design $\mathbf{X}$ in (3), $n=b_1+b_2$, $p=v$. Ceranka and Graczyk 2015 proved the following lemma.

Lemma 2. Any chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ in the form (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given in (1), is nonsingular if and only if $2k_1\neq k_2$ or $2k_1=k_2\neq v$.

The conditions given in Theorem 2 indicate that the optimality conditions and the construction methods of the regular D-optimal design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ are dependent on the parameter ρ. Thus, we obtain the following Theorem.

Theorem 3. Any nonsingular chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1), is regular D-optimal if and only if

(i) $2r_1-b_1\neq b_2-r_2$,

(ii) $b_1-4(r_1-\lambda_1)+b_2+\lambda_2-2r_2<0$ and

(iii) $\rho=\dfrac{b_1-4(r_1-\lambda_1)+b_2+\lambda_2-2r_2}{(2r_1-b_1+r_2-b_2)^2-(b_1+b_2-1)(b_1-4(r_1-\lambda_1)+b_2+\lambda_2-2r_2)}$.

Proof. For the design matrix $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ in (3) and $\mathbf{G}$ in (1), we have $\mathbf{X}^{'}\mathbf{X}=(4(r_1-\lambda_1)+r_2+2\rho_{22}-\lambda_2)\mathbf{I}_v+(b_1-4(r_1-\lambda_1)+b_2+\lambda_2-2r_2)\mathbf{1}_v\mathbf{1}_v^{'}$. From Theorem 2 it follows that chemical balance weighing design is regular D-optimal if and only if conditions (i) and (ii) hold. From $\mathbf{X}^{'}\mathbf{1}_n=\mathbf{z}_p$ we have $\mathbf{c}_j^{'}\mathbf{X}^{'}\mathbf{1}_n=m-2u$ or $-(m-2u)$, $j=1,2,...,p$, where $m-2u=2r_1-b_1+r_2-b_2$, $\mathbf{c}_j$ is jth column of the matrix $\mathbf{I}_p$. From condition $\mathbf{X}^{'}\mathbf{X}=m\mathbf{I}_p-\dfrac{\rho(m-2u)^2}{1+\rho(n-1)}(\mathbf{I}_p-\mathbf{1}_p\mathbf{1}_p^{'})$ we have $\mathbf{c}_j^{'}\mathbf{X}^{'}\mathbf{X}\mathbf{c}_j=\dfrac{\rho(m-2u)^2}{1+\rho(n-1)}$ and hence

$\mathbf{c}_j^{'}\mathbf{X}^{'}\mathbf{X}\mathbf{c}_{j^{'}} = b_1 - 4(r_1 - \lambda_1) + b_2 + \lambda_2 - 2r_2$, $j \neq j^{'}$. Then $b_1 - 4(r_1 - \lambda_1) + b_2 + \lambda_2 - 2r_2 = \frac{\rho(2r_1 - b_1 + r_2 - b_2)^2}{1 + \rho(b_1 + b_2 - 1)}$ and therefore we have (iii). Under condition (ii), the denominator (iii) is greater than zero, hence $\rho < 0$. Since (i), then $\frac{-1}{n-1} < \rho < 0.$

Below, we present the theorems that give the parameters of the balanced incomplete block designs and the ternary balanced block designs. Based on these parameters we construct the incidence matrices and next, the design matrices of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n \times p}(-1,0,1)$. Here, $p = v$ and $n = b_1 + b_2$.

Theorem 4. Let $\rho = \frac{-2}{u^2(t+1)^2 + 8us + 8u + 16s + 10}$, where $u = 1,2,...$ and $t = 1$, $s = 1,2,...$, or $t = 2$, $s = 2,3,...$, or $t = 3$, $s = 3,4,...$. If the parameters of the balanced incomplete block design are equal to $v = 4(s+1)$, $b_1 = 2(4s+3)$, $r_1 = 4s+3$, $k_1 = 2(s+1)$, $\lambda_1 = 2s+1$ and the parameters of the ternary balanced block design are equal to $v = 4(s+1)$, $b_2 = 4u(s+1)$, $r_2 = u(4s+3-t)$, $k_2 = 4s+3-t$, $\lambda_2 = 2u(2s-t+1)$, $\rho_{12} = u\left(4s+4-(t+1)^2\right)$, $\rho_{22} = 0.5ut(t+1)$, then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n \times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is as (1), is regular D-optimal.

Proof. It is evident that the parameters given above satisfy the conditions (i)–(iii) of Theorem 3.

Theorem 5. Let $\rho = \frac{-1}{8t^2 + 8s^2 + 8st + 8s + 4t + u}$, $s,t,u = 1,2,...$, $4t \geq 2s+1$. If the parameters of the balanced incomplete block design are equal to $v = (2s+1)^2$, $b_1 = 4t(2s+1)$, $r_1 = 4st$, $k_1 = s(2s+1)$, $\lambda_1 = t(2s-1)$ and the ternary balanced block design are equal to $v = k_2 = (2s+1)^2$, $b_2 = r_2 = 8s^2 + 8s + u + 1$, $\lambda_2 = 8s^2 + 8s + u - 1$, $\rho_{12} = u+1$, $\rho_{22} = 4s(4s+1)$, then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n \times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1), is regular D-optimal.

Proof. It is easy to see that the parameters given above satisfy the conditions (i)–(iii) of Theorem 3.

Theorem 6. If the parameters of the balanced incomplete block design are equal to $v = 4s+1$, $b_1 = 2(4s+1)$, $r_1 = 4s$, $k_1 = 2s$, $\lambda_1 = 2s-1$ and for a given ρ, the parameters of the ternary balanced block design are equal to

(i) $\rho = \dfrac{-1}{16s+u+3}$, $v = k_2 = 4s+1$, $b_2 = r_2 = 8s+u+1$, $\lambda_2 = 8s+u-1$, $\rho_{12} = u+1$, $\rho_{22} = 4s$, $s,u = 1,2,...$,

(ii) $\rho = \dfrac{-3}{36s+3u+7}$, $v = k_2 = 4s+1$, $b_2 = r_2 = 4s+u$, $\lambda_2 = 4s+u-1$, $\rho_{12} = u$, $\rho_{22} = 2s$, $s,u = 1,2$,

(iii) $\rho = \dfrac{-2}{u^2(t+1)^2 + 2u(2t+3) + 8s(u+2) + 6}$, $v = 4s+1$, $b_2 = u(4s+1)$, $r_2 = u(4s-t)$, $k_2 = 4s-t$, $\lambda_2 = u(4s-2t-1)$, $\rho_{12} = u\left(4s+1-(t+1)^2\right)$, $\rho_{22} = 0.5ut(t+1)$, for any $u = 1,2,...$, and moreover for the cases: the first one $t=1$, $s = 1,2,...$, except $s = u = 1$, the second one $t = 2$, $s = 3,4,...$, and the third one $t = 3$, $s = 5,6,...$,

where $4s+1$ is a prime or a prime power, then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1), is regular D-optimal.

Proof. It is a simple matter to check that the parameters given above satisfy the conditions given in Theorem 3.

Theorem 7. If the parameters of the balanced incomplete block design are equal to $v = b_1 = 4s^2-1$, $r_1 = k_1 = 2s^2-1$, $\lambda_1 = s^2-1$ and for a given ρ, the parameters of the ternary balanced block design are equal to

(i) $\rho = \dfrac{-3}{36s^2+3u-14}$, $v = k_2 = 4s^2-1$, $b_2 = r_2 = 8s^2+u-3$, $\lambda_2 = 8s^2+u-5$, $\rho_{12} = u+1$, $\rho_{22} = 2(2s^2-1)$, $s = 2,3,...$, $u = 1,2,...$,

(ii) $\rho = \dfrac{-1}{u^2(t+1)^2 + u(2t+1) + 4s^2(u+1) - 1}$, $v = 4s^2 - 1$, $b_2 = u(4s^2 - 1)$,
$r_2 = u(4s^2 - t - 2)$, $k_2 = 4s^2 - t - 2$, $\lambda_2 = u(4s^2 - 2t - 3)$, $\rho_{12} = u(4s^2 - (t+1)^2)$,
$\rho_{22} = 0.5ut(t+1)$, for any $u = 1,2,\ldots$, and $t = 1,2$, $s = 2,3,\ldots$, or $t = 3$, $s = 3,4,\ldots$,
then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1), is regular D-optimal.

Proof. It is easy to check that the parameters given above satisfy the conditions indicated in Theorem 3.

Theorem 8. If the parameters of the balanced incomplete block design are equal to $v = b_1 = 4s + 3$, $r_1 = k_1 = 2s + 1$, $\lambda_1 = s$ and for a given ρ, the parameters of the ternary balanced block design are equal to

(i) $\rho = \dfrac{-3}{36s + 3u + 22}$, $v = k_2 = 4s + 3$, $b_2 = r_2 = 8s + u + 5$, $\lambda_2 = 8s + u + 3$,
$\rho_{12} = u + 1$, $\rho_{22} = 2(2s + 1)$, $s,u = 1,2,\ldots$,

(ii) $\rho = \dfrac{-1}{u^2(t+1)^2 + u(2t+5) + 4s(u+1) + 3}$, $v = 4s + 3$, $b_2 = u(4s + 3)$,
$r_2 = u(4s - t + 2)$, $k_2 = 4s - t + 2$, $\lambda_2 = u(4s - 2t + 1)$, $\rho_{12} = u(4s + 3 - (t+1)^2)$,
$\rho_{22} = 0.5ut(t+1)$, for any $u = 1,2,\ldots$, and $t = 1$, $s = 1,2,\ldots$, or $t = 2$, $s = 2,3,\ldots$, and the third one $t = 3$, $s = 4,5,\ldots$,

where $4s + 3$ is a prime or a prime power, then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is as in (1), is regular D-optimal.

Proof. It follows directly that the parameters given above satisfy the conditions (i)-(iii) of Theorem 3.

Theorem 9. If the parameters of the balanced incomplete block design are equal to $v = b_1 = 8s + 7$, $r_1 = k_1 = 4s + 3$, $\lambda_1 = 2s + 1$ and for a given ρ, the parameters of the ternary balanced block design are equal to

(i) $\rho = \dfrac{-3}{72s + 3u + 58}$, $v = k_2 = 8s + 7$ $b_2 = r_2 = 16s + u + 13$, $\lambda_2 = 16s + u + 11$,
$\rho_{12} = u + 1$, $\rho_{22} = 2(4s + 3)$, $s,u = 1,2,\ldots$,

(ii) $\rho = \frac{-1}{u^2(t+1)^2 + u(2t+9) + 8s(u+1) + 7}$, $v = 8s+7$, $b_2 = u(8s+7)$, $r_2 = u(8s-t+6)$, $k_2 = 4s-t+6$, $\lambda_2 = u(8s-2t+5)$, $\rho_{12} = u\left(8s+7-(t+1)^2\right)$, $\rho_{22} = 0.5ut(t+1)$, for any $u = 1,2,...$, and $t = 1,2$, $s = 1,2,...$, or $t = 3$, $s = 2,3,...$, then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n \times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is as in (1), is regular D-optimal.

Proof. It is obvious that the parameters given in (i)–(ii) satisfy the three conditions presented in Theorem 3.

Theorem 10. If the parameters the ternary balanced block design are equal to $v = k_2 = 4s^2$, $b_2 = r_2 = 8s^2 + u - 2$, $\lambda_2 = 4s^2 + u - 4$, $\rho_{12} = u$, $\rho_{22} = 4s^2 - 1$ and for a given ρ, the parameters of the balanced incomplete block design are equal to

(i) $\rho = \frac{-1}{14s^2 + u - 4}$, $v = b_1 = 4s^2$, $r_1 = k_1 = s(2s+1)$, $\lambda_1 = s(s+1)$, $s,u = 1,2,...$,

(ii) $\rho = \frac{-1}{14s^2 + u - 4}$, $v = b_1 = 4s^2$, $r_1 = k_1 = s(2s-1)$, $\lambda_1 = s(s-1)$, $s = 2,3,...$, $u = 1,2,...$,

(iii) $\rho = \frac{-1}{2t^2 + 8s^2 + 4st + u - 3}$, $v = 4s^2$, $b_1 = 4st$, $r_1 = t(2s-1)$, $k_1 = s(2s-1)$, $\lambda_1 = t(s-1)$, $s,t = 2,3,...$, $t \geq s$, $u = 1,2,...$,

then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n \times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is of the form (1), is regular D-optimal.

Proof. It is clear that the parameters given above satisfy the conditions (i)–(iii) of Theorem 3.

Theorem 11. If for a given ρ, the parameters of the balanced incomplete block design and the ternary balanced block design are equal to

(i) $\rho = \frac{-1}{4u^2 + 29u + 55}$, $v = 5$, $b_1 = 10$, $r_1 = 4$, $k_1 = 2$, $\lambda_1 = 1$ and $v = 5$, $b_2 = 5(u+2)$, $r_2 = 3(u+2)$, $k_2 = 3$, $\lambda_2 = u+3$, $\rho_{12} = u+6$, $\rho_{22} = u$, $u = 1,2,...$,

(ii) $\rho = \frac{-1}{u^2+15u+65}$, $v=9$, $b_1=18$, $r_1=8$, $k_1=4$, $\lambda_1=3$ and $v=9$, $b_2=3(u+4)$, $r_2=2(u+4)$, $k_2=6$, $\lambda_2=u+5$, $\rho_{12}=8$, $\rho_{22}=u$, $u=1,2,\ldots$,

(iii) $\rho = \frac{-1}{16s^2+12s+u+7}$, $v=9$, $b_1=12s$, $r_1=4s$, $k_1=3$, $\lambda_1=s$ and $v=9$, $b_2=u+8$, $r_2=u+8$, $k_2=9$, $\lambda_2=u+7$, $\rho_{12}=u$, $\rho_{22}=4$, $s,u=1,2,\ldots$,

(iv) $\rho = \frac{-1}{4s^2+16s+61}$, $v=12$, $b_1=22$, $r_1=11$, $k_1=6$, $\lambda_1=5$ and $v=12$, $b_2=3(2s+5)$, $r_2=2(2s+5)$, $k_2=8$, $\lambda_2=2(2s+3)$, $\rho_{12}=6-2s$, $\rho_{22}=3s+2$, $s=0,1,2$,

(v) $\rho = \frac{-2}{2u+59}$, $v=15$, $b_1=15$, $r_1=7$, $k_1=7$, $\lambda_1=3$ and $v=15$, $b_2=u+14$, $r_2=u+14$, $k_2=15$, $\lambda_2=u+13$, $\rho_{12}=u$, $\rho_{22}=7$, $u=1,2,\ldots$,

then the chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ given by (3) with the variance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is as in (1), is regular D-optimal.

Proof. It is easy to see that the parameters (i)–(v) satisfy the conditions presented in the thesis of Theorem 3.

4. DISCUSSION

The issues concerning regular D-optimal chemical balance weighing designs with negative correlated errors were presented in Ceranka and Graczyk (2014c). In the mentioned manuscript, the construction of the design matrix based on the set of the incidence matrices of the balanced bipartite weighing designs was introduced. For example, in the class $\mathbf{\Phi}_{20\times 5}(-1,0,1)$, the matrix of D-optimal design was determined for $\rho = -1/55$ (Th. 2.3(xii), $s=2$, $t=1$), $\rho = -1/83$ (Th. 2.3(xiii), $s=2$, $t=1$). Furthermore, in the class $\mathbf{\Phi}_{72\times 9}(-1,0,1)$ for $\rho = -3/469$ (Th. 2.3(vi), $s=4$), $\rho = -1/199$ (Th. 2.3(x), $s=4$, $t=1$), $\rho = -1/215$ (Th. 2.3(xii), $s=4$, $t=1$), $\rho = -1/327$ (Th. 2.3(xiii), $s=4$, $t=1$), $\rho = -1/471$ (Th. 2.3(ix), $s=4$). As it can be seen, it is not possible to determine regular D-optimal chemical balance weighing design in any class $\mathbf{\Phi}_{n\times p}(-1,0,1)$ and for any value ρ. Therefore, we introduced new methods of constructing the design matrix. Due to the method considered in the present paper, we are able to determine regular D-optimal chemical balance weighing design in the class $\mathbf{\Phi}_{20\times 5}(-1,0,1)$, for $\rho = -\frac{1}{20}$ (Th. 6(i), $s = u = 1$), $\rho = -\frac{1}{37}$ (Th. 6(iii), $s = t = 1$, $u = 1$). Thereafter, in the class $\mathbf{\Phi}_{72\times 9}(-1,0,1)$ for $\rho = -\frac{1}{72}$ (Th. 6(i), $s = 2$, u= 37), $\rho = -\frac{1}{169}$ (Th. (iii), $s = 2$, $t = 1$, $u = 6$), $\rho = -\frac{1}{135}$ (Th. 11(iii), $s = 2$, $u = 40$), $\rho = -\frac{1}{199}$ (Th. 5, $s = 1$, $t = 4$, $u = 7$), $\rho = -\frac{1}{471}$ (Th. 11(ii), $u = 14$).

5. EXAMPLE

Let us consider the experiment in which we determine unknown measurements of $p = 5$ objects by use of $n = 15$ measurements assuming that the correlation between measurement errors equals $\rho = -\frac{3}{46}$ So, we construct the matrix $\mathbf{X} \in \mathbf{\Phi}_{15\times 5}(-1,0,1)$ according to the Theorem 4(iii). Thus, we take the balanced incomplete block design with the parameters $v = 5$, $b_1 = 10$, $r_1 = 4$, $k_1 = 2$, $\lambda_1 = 1$ and the ternary balanced block design with the parameters $v = b_2 = r_2 = k_2 = 5$, $\lambda_2 = 4$, $\rho_{12} = 1$, $\rho_{22} = 2$, given by the incidence matrices

$$\mathbf{N}_1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix} \text{ and } \mathbf{N}_2 = \begin{bmatrix} 1 & 2 & 0 & 0 & 2 \\ 2 & 1 & 2 & 0 & 0 \\ 0 & 2 & 1 & 2 & 0 \\ 0 & 0 & 2 & 1 & 2 \\ 2 & 0 & 0 & 2 & 1 \end{bmatrix}.$$

According to the formula (3) we form the matrix $\mathbf{X} \in \mathbf{\Phi}_{15\times 5}(-1,0,1)$ of the regular D-optimal chemical balance weighing design as

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

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O PEWNYCH WŁASNOŚCIACH I KONSTRUKCJACH UKŁADÓW DOŚWIADCZALNYCH

Streszczenie. W pracy rozważamy problematykę związaną z wyznaczeniem planu eksperymentu wykonanego zgodnie z modelem chemicznego układu wagowego przy założeniu, że błędy pomiarów są jednakowo ujemnie skorelowane. Powyższe zagadnienie rozważamy z punktu widzenia D-optymalności. Podajemy nową metodę konstrukcji D-optymalnego chemicznego układu wagowego oraz listę proponowanych planów eksperymentu.

Słowa kluczowe: chemiczny układ wagowy, D-optymalność, trójkowy zrównoważony układ bloków, układ zrównoważony o blokach niekompletnych