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New Results Regarding the Construction Method for D-optimal Chemical Balance Weighing Designs

Abstract: We study an experiment in which we determine unknown measurements of p objects in n weighing operations according to the model of the chemical balance weighing design. We determine a design which is D-optimal. For the construction of the D-optimal design, we use the incidence matrices of balance incomplete block designs, balanced bipartite weighing designs and ternary balanced block designs. We give some optimality conditions determining the relationships between the parameters of a D-optimal design and we present a series of parameters of such designs. Based on these parameters, we will be able to set down D-optimal designs in classes in which it was impossible so far.

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

JEL: C02, C18, C90

1. Introduction

In this paper, we consider the linear model

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e},$$

where:

\mathbf{y} is an $n \times 1$ random vector of observations,

$\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$ of known elements where x_{ij} equals $-1, 0$ or 1 ,

\mathbf{w} is a $p \times 1$ vector of unknown measurements of objects,

\mathbf{e} is an $n \times 1$ random vector of errors.

We assume that $E(\mathbf{e}) = \mathbf{0}_n$ and $\text{Var}(\mathbf{e}) = \sigma^2 \mathbf{I}_n$, where $\mathbf{0}_n$ is the $n \times 1$ vector with zero elements everywhere, \mathbf{I}_n denotes the identity matrix of rank n . Such form of the matrix $\text{Var}(\mathbf{e})$ indicates that errors are uncorrelated and have the same variance.

In order to estimate \mathbf{w} , we use the least squares method and the normal equations of the form $\mathbf{X}'\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{y}$. Any chemical balance weighing design is singular or non-singular, depending on whether the matrix $\mathbf{X}\mathbf{X}$ is singular or non-singular, respectively. If \mathbf{X} is of full column rank, the least squares estimator of \mathbf{w} is equal to $\hat{\mathbf{w}} = (\mathbf{M})^{-1} \mathbf{X}'\mathbf{y}$ and the covariance matrix of $\hat{\mathbf{w}}$ is given by $\text{Var}(\hat{\mathbf{w}}) = \sigma^2 (\mathbf{M})^{-1}$, where $\mathbf{M} = \mathbf{X}\mathbf{X}$ is called the information matrix for the design \mathbf{X} . In the literature, basic problems of weighing designs are discussed. Jacroux, Wong and Masaro (1983), Sathe and Shenoy (1990) gave the introduction to different optimality criteria.

Here, we consider chemical balance weighing designs under the basic assumption that the design is D-optimal. The weighing design is stated by entering its matrix. The design \mathbf{X}_D is called D-optimal in the given class $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ if $\det(\mathbf{X}'_D \mathbf{X}_D) = \max(\det(\mathbf{M}) : \mathbf{X} \in \Phi_{n \times p}(-1, 0, 1))$. Moreover, if $\det(\mathbf{M})$ attains the upper bound, then the design is called regular D-optimal. For more theory, we refer the reader to the papers of Katulska and Smaga (2013), Ceranka and Graczyk (2016).

Based on the results given in Ceranka and Graczyk (2017), we have:

Theorem 1.1. Any chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ with the variance matrix of errors $\sigma^2 \mathbf{I}_n$ is regular D-optimal if and only if $\mathbf{X}\mathbf{X} = m\mathbf{I}_p$, where m is the maximal number of elements different from zero in the j -th column, where $j = 1, \dots, p$.

The relations between the parameters of the D-optimal chemical balance weighing design imply that for any combination of numbers p and n , we are not able to determine a D-optimal design. In other words, in any class $\Phi_{n \times p}(-1, 0, 1)$, a D-optimal chemical balance weighing design may not exist.

Therefore, the aim of this paper is an investigation of a new construction method of a D-optimal chemical balance weighing design. Based on this method, we will be able to set down D-optimal designs in classes in which it was impossible so far. Thus, we can determine estimators of unknown parameters having the smallest possible product of its variances.

We construct the design matrix of the D-optimal chemical balance weighing design by use of incidence matrices of known block designs. Here we take the incidence matrices of the balanced incomplete block design, the balanced bipartite weighing design and the ternary balanced block design. New matrix construction methods will allow us to determine the D-optimal chemical balance weighing design for new combinations of the number of objects and the number of measurements which are not known in the literature. The properties of mentioned designs are presented in Section 2, whereas Section 3 contains the methods of construction of the design matrix. Finally, some examples of experimental plans are given.

2. Balanced block design

In this section, we present the definition and properties of the balanced incomplete block design given in Raghavarao (1971), the balanced bipartite weighing design given in Huang (1976) and the ternary balanced block design given in Billington (1984).

A balanced incomplete block design (BIBD) with the parameters v, b, r, k, λ is an arrangement of v treatments into b blocks, each of size k . Each treatment occurs at most once in each block, occurs in exactly r blocks, and every pair of treatments occurs together in exactly λ blocks. Let N be the incidence matrix of a balanced incomplete block design. The parameters are related by the following identities $vr = bk, \lambda(v-1) = r(k-1), NN' = (r-\lambda)I_v + \lambda I_v I_v'$, where I_v is $v \times 1$ vector of ones.

A balanced bipartite weighing design (BBWD) with the parameters $v, b, r, k_1, k_2, \lambda_1, \lambda_2$ is an arrangement of v treatments into b blocks. Each block containing k distinct treatments is divided into 2 subblocks containing k_1 and k_2 treatments, respectively, where $k = k_1 + k_2$. Each treatment appears in r blocks. Every pair of treatments from different subblocks appears together in λ_1 blocks and every pair of treatments from the same subblocks appears together in λ_2 blocks. Let N^* be the incidence matrix of such a design. The parameters are not independent and they are related by the following equalities

$$vr = bk, b = \frac{\lambda_1 v(v-1)}{2k_1 k_2}, \lambda_2 = \frac{\lambda_1 [k_1(k_1-1) + k_2(k_2-1)]}{2k_1 k_2}, r = \frac{\lambda_1 k(v-1)}{2k_1 k_2},$$

$$N^* N^{*'} = (r - \lambda_1 - \lambda_2) I_v + (\lambda_1 + \lambda_2) I_v I_v'$$

A ternary balanced block design (TBBD) with the parameters $v, b, r, k, \lambda, \rho_1, \rho_2$ is an arrangement of v treatments in b blocks each of size k . Each treatment appears 0, 1, 2 times in a given block, repeated r times. Each of the distinct pairs of treatments occurs λ times. Each element appears once in ρ_1 block and twice in ρ_2 blocks, where ρ_1 and ρ_2 are a known constant for the design. Let \mathbf{N} be the incidence matrix of a ternary balanced block design. The following relations are satisfied

$$vr = bk, r = \rho_1 + 2\rho_2, \lambda(v-1) = \rho_1(k-1) + 2\rho_2(k-2) = r(k-1) - 2\rho_2,$$

$$\mathbf{N}\mathbf{N}' = (\rho_1 + 4\rho_2 - \lambda)\mathbf{I}_v + \lambda\mathbf{1}_v\mathbf{1}_v' = (r + 2\rho_2 - \lambda)\mathbf{I}_v + \lambda\mathbf{1}_v\mathbf{1}_v'$$

3. Construction

A large number of publications presenting construction methods of optimal chemical balance weighing designs can be found in the literature. Generally, the construction methods are based on the incidence matrices of known block designs, see Ceranka and Graczyk (2018), Graczyk and Janiszewska (2019). When we determine the design matrix of the D-optimal chemical balance weighing design, then we prepare a plan of an experiment in which we determine unknown measurements of p objects by using n measurement operations.

Let \mathbf{N}_1 be the incidence matrix of BIBD with the parameters $v, b_1, r_1, k_1, \lambda_1$. Moreover, let \mathbf{N}_2^* be the incidence matrix of BBWD with the parameters $v, b_2, r_2, k_{12}, k_{22}, \lambda_{12}, \lambda_{22}$. Based on the matrix \mathbf{N}_2^* , we form the matrix \mathbf{N}_2 by replacing k_{12} elements equal to +1 in each column which corresponds to the elements belonging to the first subblock by -1. Consequently, each column of \mathbf{N}_2 will contain k_{12} elements equal to -1, k_{22} elements equal to 1 and $v - k_{12} - k_{22}$ elements equal to 0. Furthermore, let \mathbf{N}_3 be the incidence matrix of TBBD with the parameters $v, b_3, r_3, k_3, \lambda_3, \rho_{13}, \rho_{23}$. Then, the design matrix $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ has the form

$$\mathbf{X} = \begin{bmatrix} 2\mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' \\ \mathbf{N}_2' \\ \mathbf{N}_3' - \mathbf{1}_{b_3}\mathbf{1}_v' \end{bmatrix}. \tag{3.1}$$

Each of the $p = v$ objects is weighed $m = b_1 + r_2 + b_3 - \rho_{13}$ times in $n = b_1 + b_2 + b_3$ measuring operations.

From Graczyk and Janiszewska (2019), we have:

Lemma 3.1. Any chemical balanced weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ given in (3.1) is non-singular if and only if $2k_1 \neq v$ or $v \neq k_3$ or $2k_1 \neq k_3$ or $k_{12} \neq k_{22}$.

Theorem 3.1. Any non-singular chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1,0,1)$ given in (3.1) is regular D-optimal if and only if

$$b_1 - 4(r_1 - \lambda_1) + \lambda_{22} - \lambda_{12} + b_3 - 2r_3 + \lambda_3 = 0. \tag{3.2}$$

In particular, the equality (3.2) is true, when any combination of these parameters which in total gives zero is true. Based on the series of parameters given by Raghavaro (1971), Huang (1976), Billington (1984), and Ceranka and Graczyk (2004a; 2004b) of the block designs presented in Section 2, we formulate the following corollaries.

Corollary 3.1. Let $v = 4s + 1$. The existence of the balanced incomplete block design with the parameters $b_1 = 2(4s + 1)$, $r_1 = 4s$, $k_1 = 2s$, $\lambda_1 = 2s - 1$ and the balanced bipartite weighing design with the parameters

$$(i) \quad b_2 = s(4s + 1), r_2 = 8s, k_{12} = 2, k_{22} = 6, \lambda_{12} = 6, \lambda_{22} = 8,$$

$$(ii) \quad b_2 = 2s(4s + 1), r_2 = 10s, k_{12} = 1, k_{22} = 4, \lambda_{12} = 6, \lambda_{22} = 8$$

and the ternary balanced block design with the parameters

$$\begin{aligned} b_3 &= u(4s + 1), r_3 = u(4s - t), k_3 = 4s - t, \lambda_3 = u(4s - 2t - 1), \\ \rho_{13} &= u(4s - t(t + 2)), \rho_{23} = 0.5tu(t + 1), \\ t &= 1, 2, 3, u, s = 1, 2, \dots, 4s > t(t + 2), \end{aligned}$$

$4s + 1$ is a prime or a prime power, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1,0,1)$ in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

Corollary 3.2. Let $v = 4(s + 1)$. The existence of the balanced incomplete block design with the parameters $b_1 = 2(4s + 3)$, $r_1 = 4s + 3$, $k_1 = 2(s + 1)$, $\lambda_1 = 2s + 1$ and the balanced bipartite weighing design with the parameters

$$b_2 = 4(s + 1)(4s + 3), r_2 = 7(4s + 3), k_{12} = 2, k_{22} = 5, \lambda_{12} = 20, \lambda_{22} = 22$$

and the ternary balanced block design with the parameters

$$\begin{aligned} b_3 &= 4u(s + 1), r_3 = u(4s - t + 3), k_3 = 4s - t + 3, \lambda_3 = 2u(2s - t + 1), \\ \rho_{13} &= u(4s - (t - 1)(t + 3)), \rho_{23} = 0.5ut(t + 1), \\ t &= 1, 2, 3, u, s = 1, 2, \dots, 4s > (t - 1)(t + 3), \end{aligned}$$

$4s + 1$ is a prime or a prime power, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

In the special case when $s = t = u = 1$, we obtain the Corollary 3.14 (Graczyk, Janiszewska, 2019).

Corollary 3.3. Let $v = 4s + 3$. The existence of the balanced incomplete block design with the parameters $b_1 = 4s + 3$, $r_1 = 2s + 1$, $k_1 = 2s + 1$, $\lambda_1 = s$ and the balanced bipartite weighing design with the parameters

$$b_2 = (2s + 1)(4s + 3), r_2 = 7(2s + 1), k_{12} = 2, k_{22} = 5, \lambda_{12} = 10, \lambda_{22} = 11$$

and the ternary balanced block design with the parameters

$$\begin{aligned} (i) \quad & b_3 = u(4s + 3), r_3 = u(4s - t + 2), k_3 = 4s - t + 2, \lambda_3 = u(4s - 2t + 1), \\ & \rho_{13} = u(4s - t^2 - 2t + 2), \rho_{23} = 0.5ut(t + 1), \\ (ii) \quad & b_3 = 2u(4s + 3), r_3 = 8u(s + 1), k_3 = 4(s + 1), \\ & \lambda_3 = 2u(4s + 5), \rho_{13} = 4u(2s + 1), \rho_{23} = 2u \end{aligned}$$

$t = 1, 2, 3, u, s = 1, 2, \dots, 4s > t(t + 2)$, $4s + 3$ is a prime or a prime power, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

In the special case when $s = t = u = 1$, we obtain the Corollary 3.7 (Graczyk, Janiszewska, 2019), when $s = 3, t = u = 1$, we obtain the Corollary 3.31 (ii) (Graczyk, Janiszewska, 2019).

Corollary 3.4. Let $v = 8s + 7$. The existence of the balanced incomplete block design with the parameters

$$b_1 = 8s + 7, r_1 = 4s + 3, k_1 = 4s + 3, \lambda_1 = 2s + 1$$

and the balanced bipartite weighing design with the parameters

$$b_2 = (8s + 7)(4s + 3), r_2 = 7(4s + 3), k_{12} = 2, k_{22} = 5, \lambda_{12} = 10, \lambda_{22} = 11$$

and the ternary balanced block design with the parameters

$$\begin{aligned} (i) \quad & b_3 = u(8s + 7), r_3 = u(8s - t + 6), k_3 = 8s - t + 6, \lambda_3 = u(8s - 2t + 5), \\ & \rho_{13} = u(8s - t^2 - 2t + 6), \rho_{23} = 0.5ut(t + 1) \end{aligned} \quad ,$$

$$(ii) \ b_3 = 2u(8s + 7), \ r_3 = 16u(s + 1), \ k_3 = 8(s + 1), \ \lambda_3 = 2u(8s + 9),$$

$$\rho_{13} = 4u(4s + 3), \ \rho_{23} = 2u$$

where $t = 1, 2, 3, u = 1, 2, \dots, s = 2, 3, \dots$, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

In the special case when $s = t = u = 1$, we obtain the Corollary 3.31 (ii) (Graczyk, Janiszewska, 2019).

Corollary 3.5. Let $v = (2s + 1)^2$. The existence of the balanced incomplete block design with the parameters $b_1 = 4u(2s + 1), r_1 = 4su, k_1 = s(2s + 1), \lambda_1 = u(2s - 1)$ and the balanced bipartite weighing design with the parameters

$$(i) \ b_2 = s(s + 1)(2s + 1)^2, \ r_2 = 8s(s + 1), \ k_{12} = 2, \ k_{22} = 6, \ \lambda_{12} = 6, \ \lambda_{22} = 8,$$

$$(ii) \ b_2 = 2s(s + 1)(2s + 1)^2, \ r_2 = 10s(s + 1), \ k_{12} = 1, \ k_{22} = 4, \ \lambda_{12} = 4, \ \lambda_{22} = 6,$$

and the ternary balanced block design with the parameters

$$b_3 = 8s(s + 1) + t + 1, \ r_3 = 8s(s + 1) + t + 1, \ k_3 = (2s + 1)^2, \ \lambda_3 = 8s(s + 1) + t - 1,$$

$$\rho_{13} = t + 1, \ \rho_{23} = 4s(s + 1), \ 4u \geq 2s + 1$$

$u, s, t = 1, 2, \dots$, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

Corollary 3.6. Let $v = 4s^2$. The existence of the balanced incomplete block design with the parameters

$$(i) \ b_1 = 4s^2, \ r_1 = s(2s - 1), \ k_1 = s(2s - 1), \ \lambda_1 = s(s - 1),$$

$$(ii) \ b_1 = 4s^2, \ r_1 = s(2s + 1), \ k_1 = s(2s + 1), \ \lambda_1 = s(s + 1),$$

$$(iii) \ b_1 = 4st, \ r_1 = t(2s - 1), \ k_1 = s(2s - 1), \ \lambda_1 = t(s - 1),$$

and the balanced bipartite weighing design with the parameters

$$b_2 = 4s^2(4s^2 - 1), \ r_2 = 7(4s^2 - 1), \ k_{12} = 2, \ k_{22} = 5, \ \lambda_{12} = 20, \ \lambda_{22} = 22$$

and the ternary balanced block design with the parameters

$$(i) \ b_3 = 2(8s^2 + 1), \ r_3 = 2(8s^2 + 1), \ k_3 = 4s^2, \ \lambda_3 = 16s^2, \\ \rho_{13} = 4(2s^2 + 1), \ \rho_{23} = 4s^2 - 1,$$

$$(ii) \ b_3 = 2(8s^2 - 3), \ r_3 = 2(8s^2 - 3), \ k_3 = 4s^2, \ \lambda_3 = 8(2s^2 - 1), \\ \rho_{13} = 4(2s^2 - 1), \ \rho_{23} = 4s^2 - 1$$

$$(iii) \ b_3 = 16s^2, \ r_3 = 16s^2, \ k_3 = 4s^2, \ \lambda_3 = 2(8s^2 - 1), \ \rho_{13} = 2(4s^2 + 1), \ \rho_{23} = 4s^2 - 1,$$

$$(iv) \ b_3 = 4(4s^2 + 1), \ r_3 = 4(4s^2 + 1), \ k_3 = 4s^2, \ \lambda_3 = 2(8s^2 + 1), \\ \rho_{13} = 2(4s^2 + 3), \ \rho_{23} = 4s^2 - 1$$

$$(v) \ b_3 = 2(4s^2 - 1) + u, \ r_3 = 2(4s^2 - 1) + u, \ k_3 = 4s^2, \\ \lambda_3 = 4(2s^2 - 1) + u, \ \rho_{13} = u, \ \rho_{23} = 4s^2 - 1,$$

$$(vi) \ b_3 = 2(8s^2 - 1), \ r_3 = 2(8s^2 - 1), \ k_3 = 4s^2, \\ \lambda_3 = 4(4s^2 - 1), \ \rho_{13} = 8s^2, \ \rho_{23} = 4s^2 - 1,$$

where $s = 1, 2, \dots$, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

Corollary 3.7. Let $v = (2s + 1)^2$. The existence of the balanced incomplete block design with the parameters $b_1 = 4u(2s + 1)$, $r_1 = 4su$, $k_1 = s(2s + 1)$, $\lambda_1 = u(2s - 1)$ and the balanced bipartite weighing design with the parameters

$$(i) \ b_2 = u(s + 1)(2s + 1)^2, \ r_2 = 5s(s + 1), \ k_{12} = 1, \ k_{22} = 4, \ \lambda_{12} = 2, \ \lambda_{22} = 3,$$

$$(ii) \ b_2 = 2s(s + 1)(2s + 1)^2, \ r_2 = 14s(s + 1), \ k_{12} = 2, \ k_{22} = 5, \ \lambda_{12} = 10, \ \lambda_{22} = 11,$$

and the ternary balanced block design with the parameters

$$(i) \ b_3 = 2(2s + 1)^2, \ r_3 = 8s(s + 1), \ k_3 = 4s(s + 1), \\ \lambda_3 = 8s^2 + 8s - 3, \ \rho_{13} = 4s(s + 1), \ \rho_{23} = 2s(s + 1),$$

$$(ii) \ b_3 = (2s + 1)^2, \ r_3 = (2s + 1)^2, \ k_3 = (2s + 1)^2, \\ \lambda_3 = 2(2s^2 + 2s + 1), \ \rho_{13} = 1, \ \rho_{23} = 2s^2 + 2s + 1$$

$$(iii) b_3 = (2s+1)^2, r_3 = 2s^2 + 2s + 3, k_3 = 2s^2 + 2s + 3, \\ \lambda_3 = s^2 + s + 2, \rho_{13} = 2s^2 + 2s + 1, \rho_{23} = 2,$$

$4u \geq 2s + 1, u, s, t = 1, 2, \dots$, implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$, in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

Corollary 3.8. Let $v = 4s^2$. The existence of the balanced incomplete block design with the parameters

$$(i) b_1 = 4s^2, r_1 = s(2s-1), k_1 = s(2s-1), \lambda_1 = s(s-1), \\ (ii) b_1 = 4s^2, r_1 = s(2s+1), k_1 = s(2s+1), \lambda_1 = s(s+1), \\ (iii) b_1 = 4st, r_1 = t(2s-1), k_1 = s(2s-1), \lambda_1 = t(s-1),$$

and the balanced bipartite weighing design with the parameters

$$b_2 = 2s^2w(4s^2 - 1), r_2 = 2w(4s^2 - 1), k_{12} = 1, k_{22} = 3, \lambda_{12} = 3w, \lambda_{22} = 3w$$

and the ternary balanced block design with the parameters

$$(i) b_3 = 4us^2, r_3 = u(4s^2 - t - 1), k_3 = 4s^2 - t - 1, \\ \lambda_3 = u(4s^2 - 2(t+1)), \rho_{13} = u(4s^2 - (t+1)^2), \rho_{23} = 0.5ut(t+1),$$

if $t = 1, 2$ then $s = 2, 3, \dots$, if $t = 3$ then $s = 3, 4, \dots, u, w = 1, 2, \dots$,

$$(ii) b_3 = 8su, r_3 = 4u(2s-1), k_3 = 2s(2s-1), \\ \lambda_3 = 8u(s-1), \rho_{13} = 2u(s-1), \rho_{23} = 2s^2 + 2s + 1, \\ (iii) b_3 = 16s^2, r_3 = 4(4s^2 + 1), k_3 = 4s^2 + 1, \\ \lambda_3 = 4(4s^2 + 3), \rho_{13} = 4(4s^2 - 1), \rho_{23} = 4, \\ (iv) b_3 = 8s^2, r_3 = 2(4s^2 + 1), k_3 = 4s^2 + 1, \\ \lambda_3 = 2(4s^2 + 2), \rho_{13} = 2(4s^2 - 1), \rho_{23} = 2, \\ (v) b_3 = 8s^2 + u - 2, r_3 = 8s^2 + u - 2, k_3 = 4s^2, \\ \lambda_3 = 8s^2 + u - 4, \rho_{13} = u, \rho_{23} = 4s^2 - 1,$$

$s, u, w = 1, 2, \dots$ implies the existence of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ in (3.1) with the variance matrix of errors $\sigma^2 \mathbf{I}_n$.

4. Examples

Let us consider an experiment in which we determine unknown measurements of $p = 5$ objects and $n = 30$ measurements. According to the Theorem 3.3, we consider the balanced incomplete block design with the parameters $v = 5$, $b_1 = 10$, $r_1 = 4$, $k_1 = 2$, $\lambda_1 = 1$ and the incidence matrix \mathbf{N}_1 , the balanced bipartite weighing design with the parameters $v = 5$, $b_2 = r_2 = 5$, $k_{12} = 1$, $k_{22} = 4$, $\lambda_{12} = 2$, $\lambda_{22} = 3$ and the incidence matrix \mathbf{N}_2^* , and also the ternary balanced block design with the parameters $v = 5$, $b_3 = 15$, $r_3 = 9$, $k_3 = 3$, $\lambda_3 = 4$, $\rho_{13} = 7$, $\rho_{23} = 1$ and the incidence matrix \mathbf{N}_3 , where

$$\mathbf{N}_1 = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{N}_2^* = \begin{bmatrix} 1_1 & 1_2 & 1_2 & 1_2 & 1_2 \\ 1_2 & 1_1 & 1_2 & 1_2 & 1_2 \\ 1_2 & 1_2 & 1_1 & 1_2 & 1_2 \\ 1_2 & 1_2 & 1_2 & 1_1 & 1_2 \\ 1_2 & 1_2 & 1_2 & 1_2 & 1_1 \end{bmatrix},$$

$$\mathbf{N}_3 = \begin{bmatrix} 2 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 & 0 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 2 & 1 & 1 \\ 0 & 0 & 0 & 2 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

Here, 1_h denotes the element belonging to the h -th subblock, $h = 1, 2$. Thus, the design matrix of the regular D-optimal chemical balance weighing design $\mathbf{X} \in \Phi_{n \times p}(-1, 0, 1)$ is given in the form

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

5. Discussion

Chemical balanced weighing designs are considered in the literature as experimental plans in the studies in which we determine unknown measurements of p objects in n measurement operations. Determining D-optimal designs, we set down the estimators of parameters with the smallest possible product of variances of the

estimator. The design matrix is interpreted as a plan of an experiment and it sets the allocation of objects to particular weighing. From this point of view, the parameters presented in corollaries 3.1–3.8 allow us to construct the incidence matrices of block designs and simultaneously experimental plans with the required properties. Given this interpretation and for different optimality criteria, the application of chemical balance weighing designs in economic research is presented in Banerjee (1975) and Ceranka and Graczyk (2014). The applications of such designs are not limited to only one field of science. In addition, these types of experiments are used in agricultural experimental practice. A detailed description of the applications was given in Ceranka and Katulska (1987) and Graczyk (2013).

It is worth emphasising that other optimality criteria are also considered in the literature. For example, detailed research on A-optimal chemical balance weighing designs is given in Ceranka and Graczyk (2015).

References

- Banerjee K.S. (1975), *Weighing Designs for Chemistry, Medicine, Economics, Operations Research, Statistics*, Marcel Dekker Inc., New York.
- Billington E.J. (1984), *Balanced n-array designs: a combinatorial survey and some new results*, "Ars Combinatoria", no. 17A, pp. 37–72.
- Ceranka B., Graczyk M. (2004a), *Balanced ternary block designs under the certain condition*, "Colloquium Biometricum", no. 34, pp. 63–75.
- Ceranka B., Graczyk M. (2004b), *Balanced bipartite weighing designs under the certain condition*, "Colloquium Biometricum", no. 34a, pp. 17–28.
- Ceranka B., Graczyk M. (2014), *On certain A-optimal biased spring balance weighing designs*, "Statistics in Transition new series", Spring, vol. 15(2), pp. 317–326.
- Ceranka B., Graczyk M. (2015), *Construction method of A-optimal chemical balance weighing designs*, "Acta Universitatis Lodzianensis. Folia Oeconomica", vol. 3(314), pp. 43–51, <http://doi.org/10.18778/0208-6018.314.06>
- Ceranka B., Graczyk M. (2016), *New construction of D-optimal weighing design with non-negative correlations of errors*, "Colloquium Biometricum", no. 46, pp. 31–45.
- Ceranka B., Graczyk M. (2017), *Some D-optimal chemical balance weighing designs: theory and examples*, "Biometrical Letters", no. 54, pp. 137–154.
- Ceranka B., Graczyk M. (2018), *Regular D-optimal weighing design with non-negative correlations of errors constructed from same block designs*, "Colloquium Biometricum", no. 48, pp. 1–17.
- Ceranka B., Katulska K. (1987), *Zastosowanie optymalnych sprężynowych układów wagowych*, [w:] *Siedemnaście Colloquium Metodologiczne z Agro-Biometrii*, PAN, Warszawa, pp. 98–108.
- Graczyk M. (2013), *Some applications on weighing designs*, "Biometrical Letters", vol. 50(1), pp. 15–26.
- Graczyk M., Janiszewska M. (2019), *Remarks about construction methods about D-optimal chemical balance weighing designs*, "Biometrical Letters" [to appear].
- Huang Ch. (1976), *Balanced bipartite block design*, "Journal of Combinatorial Theory (A)", no. 21, pp. 20–34.
- Jacroux M., Wong C.S., Masaro J.C. (1983), *On the optimality of chemical balance weighing design*, "Journal of Statistical Planning and Inference", no. 8, pp. 213–240.



- Katulska K., Smaga Ł. (2013), *A note on D-optimal chemical balance weighing designs and their applications*, "Colloquium Biometricum", no. 43, pp. 37–45.
- Raghavarao D. (1971), *Constructions and Combinatorial Problems in designs of Experiments*, John Wiley Inc., New York.
- Sathe Y.S., Shenoy R.G. (1990), *Construction method for some A- and D-optimal weighing designs when $N \equiv 3(mod 4)$* , "Journal of Statistical Planning and Inference", no. 24, pp. 369–375.

Nowe wyniki dotyczące metody konstrukcji D- optymalnych chemicznych układów wagowych

Streszczenie: W artykule rozważamy doświadczenie, w którym wyznaczamy nieznaną miarę p obiektów przy użyciu n operacji pomiarowych zgodnie z modelem chemicznego układu wagowego. Wyznaczamy układ, który spełnia kryterium D- optymalności. Do konstrukcji D- optymalnego układu wykorzystujemy macierze incydencji układów zrównoważonych o blokach niekompletnych, dwudzielne układy blokowe oraz trójkowe zrównoważone układy blokowe. Podajemy pewne warunki optymalności, określające zależności między parametrami D- optymalnego układu i prezentujemy serie parametrów takich układów. Na podstawie tych parametrów będziemy mogli wyznaczyć D- optymalne układy w klasach, w których do tej pory nie było to możliwe.

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

JEL: C02, C18, C90

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