A C T A   U N I V E R S I T A T I S   L O D Z I E N S I S
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# NOTES ABOUT SINGULAR CHEMICAL BALANCE WEIGHING DESIGN

**Abstract.** In the paper we consider singular chemical balance weighing design and we give the method of construction of nonsingular design based on the singular one. The construction method of the design matrix of the chemical balance weighing design is based on the incidence matrices of the ternary balanced block design.

**Key words:** chemical balance weighing design, singular design, ternary balanced block design.

## I. INTRODUCTION

The chemical balance weighing design we define as a design which is determined by the model $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where

1) $\mathbf{y}$ is an $n \times 1$ random observed vector of the recorded results of weights,

2) $\mathbf{X} = (x_{ij})$ is the design matrix of the chemical balance weighing design with elements equal to –1, 0 or 1, $i = 1,2,...,n$, $j = 1,2,..., p$,

3) $\mathbf{w}$ is a $p \times 1$ vector representing unknown weights of objects,

5) $\mathbf{e}$ is an $n \times 1$ random vector of errors,

6) $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and $\mathrm{Var}(\mathbf{e}) = \sigma^2 \mathbf{I}_n$.

The normal equations estimating $\mathbf{w}$ are of the form

$$\mathbf{X}'\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{y}, \qquad (1)$$

where $\hat{\mathbf{w}}$ is the vector of the weights estimated by the least squares method. We said that any chemical balance weighing design is singular or not singular

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depending on whether the matrix $\mathbf{X}'\mathbf{X}$ is singular or not singular, respectively. Now, if $\mathbf{X}$ is of full column rank the least squares estimates of $\mathbf{w}$ are given by $\hat{\mathbf{w}} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}$ and the variance matrix of $\hat{\mathbf{w}}$ is $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\left(\mathbf{X}'\mathbf{X}\right)^{-1}$. In the case when $\mathbf{X}$ is not of full column rank then (1) is resolvable and we are not able to estimate unknown measurements of objects. Hence, in the present paper we propose to add one additionally measurement operation in order to receive nonsingular design matrix $\mathbf{X}$.

## II. THE DESIGN MATRIX

Now, we give the definition of the ternary balanced block design presented in Billington (1984).

A ternary balanced block design is defined as the design in which

1) we place $v$ treatments in $b$ blocks, each of the size $k$,
2) each treatment occurs $r$ times altogether and 0, 1 or 2 times in each block,
3) each of the distinct pairs of elements appear $\lambda$ times,
4) each treatment occurs once in $\rho_1$ blocks and twice in $\rho_2$ blocks, where $\rho_1$ and $\rho_2$ are constant for the design,
5) **N** is the incidence matrix of the ternary balanced block design,
6) the parameters are connected by the following equalities

$$vr = bk,$$

$$r = \rho_1 + 2\rho_2, \tag{2}$$

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

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

**Definition 1.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ is optimal if $\mathrm{Var}(\hat{w}_j)$ attains the lower bound for each $j$, $j = 1,2,...,p$.

**Theorem 1.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ is optimal if and only if

$$\mathbf{X}^{'}\mathbf{X} = m\mathbf{I}_p \,, \tag{3}$$

where $m$ denotes the maximum number of elements equal to –1 or 1 in the columns of the design matrix $\mathbf{X}$ .

Let us consider the incidence matrix $\mathbf{N}$ of the ternary balanced block designs with the parameters $v, b, r, k, \lambda, \rho_1, \rho_2$. We form the matrix

$$\mathbf{X} = \mathbf{N}^{'} - \mathbf{1}_b\mathbf{1}_v^{'} \,. \tag{4}$$

From Ceranka and Graczyk (2000) we have

**Lemma 2.1.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (4) is nonsingular if and only if

$$v \neq k \,. \tag{5}$$

Let note, the condition (5) is equivalent to the condition $b \neq r$.

**Theorem 2.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (4) is optimal if and only if

$$b + \lambda - 2r = 0 \tag{6}$$

Some construction methods and series of parameters of the ternary balanced block designs leading to the optimum chemical balance weighing design in the case when $\mathbf{X}$ given in (4) is nonsingular are given in Ceranka and Graczyk (2000), (2004a). Now, we consider the case when the design matrix $\mathbf{X}$ given in (4) is singular, i.e. the parameters of the ternary balanced block design satisfy the condition $v = k \quad (b = r)$.

Let us consider the design matrix $\mathbf{X}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{N}^{'} - \mathbf{1}_b\mathbf{1}_v^{'} \\ \mathbf{x}^{'} \end{bmatrix}, \ \mathbf{x} = \left(x_\varsigma\right), x_\varsigma = \begin{cases} +1 \ \text{or} \ -1 & \text{for} \quad \varsigma = 1,2,...,s \\ 0 & \text{for} \quad \varsigma = s+1,...,v \end{cases}. \tag{7}$$

For the design matrix $\mathbf{X}$ in the form (7) we have $\mathbf{X}'\mathbf{X} = \begin{bmatrix} a\mathbf{I}_s + (d+1)\mathbf{1}_s\mathbf{1}_s' & d\mathbf{1}_s\mathbf{1}_{v-s}' \\ d\mathbf{1}_{v-s}\mathbf{1}_s' & a\mathbf{I}_{v-s} + d\mathbf{1}_{v-s}\mathbf{1}_{v-s}' \end{bmatrix}$, where $d = \lambda - r$, $a = 2\rho_2 - d$. From optimality condition (3) it derivers that $d = 0$ and simultaneously $d + 1 = 0$. Then we become contradiction. Thus we have

**Theorem 3.** Optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (7) doesn't exist.

Let us consider the design matrix $\mathbf{X}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v' \\ \mathbf{x}' \end{bmatrix}, \ \mathbf{x} = (x_\varsigma), \quad x_\varsigma = +1 \text{ or } -1, \quad \varsigma = 1,2,...,v. \tag{8}$$

For the design matrix $\mathbf{X}$ in the form (8) we have

$$\mathbf{X}'\mathbf{X} = a\mathbf{I}_v + (d+1)\mathbf{1}_v\mathbf{1}_v', \tag{9}$$

and $\det(\mathbf{X}'\mathbf{X}) = va^{v-1}$. Because $a \neq 0$ then $\det(\mathbf{X}'\mathbf{X}) \neq 0$. Hence

**Theorem 4.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (8) is nonsingular.

**Theorem 5.** Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (8) is optimal if and only if $r = \lambda + 1$.

Proof. We become the thesis comparing the condition (3) and the form (9).

Based on the papers Billington and Robinson (1983), Ceranka and Graczyk (2004b) and taking into account the relations between the parameters of the ternary balanced block designs we are able to formulate

**Theorem 6.** If the parameters of the ternary balanced block design are equal to $v = k = 2\rho_2 + 1$, $b = r = \lambda + 1$, $\lambda$, $\rho_1 = \lambda - 2\rho_2 + 1$, $\rho_2$ then the chemical balance weighing design with the design matrix $\mathbf{X}$ given in (8) is optimal.

Proof. It is obvious that for given parameters and the design matrix in the form (8) condition (3) is true.

## III. EXAMPLE

Let us consider the ternary balanced block design with the parameters $v = k = b = r = 3, \lambda = 2, \quad \rho_1 = \rho_2 = 1$ given by the incidence matrix $\mathbf{N} = \begin{bmatrix} 2 & 0 & 1 \\ 1 & 2 & 0 \\ 0 & 1 & 2 \end{bmatrix}$. For the design matrix $\mathbf{X}$ in the form (4) we have $\mathbf{X} = \begin{bmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$ and $\det\left(\mathbf{X}'\mathbf{X}\right) = 0$. But if we will consider the design matrix $\mathbf{X}$ in the form (8) for $\mathbf{x}' = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$ we have

$$\mathbf{X} = \begin{bmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}, \tag{10}$$

and $\det\left(\mathbf{X}'\mathbf{X}\right) \neq 0$. Based on the Theorem 5 the chemical balance weighing design with the design matrix in (10) is optimal.

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**UWAGI O OSOBLIWYCH CHEMICZNYCH UKŁADACH WAGOWYCH**

W literaturze omawiającej zagadnienia optymalnej estymacji nieznanych miar obiektów w modelu chemicznego układu wagowego przyjmuje się założenie, że układ jest nieosobliwy. Autorzy w pracy odpowiadają na pytanie co zrobić, gdy macierz układu nie jest macierzą pełnego rzędu kolumnowego.