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A FEW REMARKS ABOUT OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS

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Summary

In the paper, singular chemical balance weighing design is considered. The method of construction of the nonsingular design based on singular one is given.

Key words and phrases: balanced bipartite weighing design, optimum chemical balance weighing design

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1. Introduction

Any chemical balance weighing design is defined as a design in which we determine unknown measurements of p objects in n measurement operations according to the model

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

where

1) $\mathbf{y}$ is a $n \times 1$ random vector of the recorded results of measurements,

2) $\mathbf{X} = (x_{ij})$, $i = 1,2,...,n$, $j = 1,2,..., p$, is the design matrix with elements $x_{ij} = +1, -1$ or 0,

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

4) $\mathbf{e}$ is an $n \times 1$ random vector of errors, $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and $\mathrm{E}(\mathbf{ee}') = \sigma^2 \mathbf{I}_n$, $\mathbf{0}_n$ is an $n \times 1$ null vector, $\mathbf{I}_n$ is the identity matrix of order n.

The normal equations estimating $\mathbf{w}$ are of the form $\mathbf{X}'\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{y}$, where $\hat{\mathbf{w}}$ is the vector estimated by the least squares method. Any chemical balance weighing design is said to be singular or not singular depending on whether the matrix $\mathbf{X}'\mathbf{X}$ is singular or not singular, respectively. If $\mathbf{X}$ is of full column rank than the least squares estimator of $\mathbf{w}$ is given by $\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ and the covariance matrix of $\hat{\mathbf{w}}$ is equal $\mathrm{V}(\hat{\mathbf{w}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1}$.

In many papers, for example, Banerjee (1975), Katulska (1984), Ceranka and Katulska (1999), Ceranka and Graczyk (2002), the chemical balance weighing designs are considered and some examples of applying these designs in the agricultural experiments are presented. In these papers, for a given number p of objects and n measurement operations, some methods of construction of the optimum chemical balance weighing designs are presented. Unfortunately, not for each combination of p and n we are able to construct optimal design having required properties. The problems are connected with relations between the parameters of the design or sometimes the design matrix is singular. Concurrently, in order to estimate all unknown measurements of objects, the design matrix must be of full column rank. In this paper we show, how to solve the problem when the chemical balance weighing design is singular.

2. The design matrix of the chemical balance weighing design

Let $\mathbf{X}$ be the design matrix of the chemical balance weighing design and let $m = \max\{m_1, m_2, ..., m_p\}$, where m_j, $(j = 1,2,..., p)$, is the number of nonzero elements in the j th column of $\mathbf{X}$. The restriction follows from m is very important in situation when some objects could be destroyed between measurements or the number of combinations between parameters is too large.

From Ceranka and Graczyk (2002) we have

Definition 2.1 Any chemical balance weighing design $\mathbf{X}$ is said to be optimum if it estimates each of unknown measurements of objects with minimum variance, i.e.

$$\mathrm{Var}(\hat{w}_j) = \frac{\sigma^2}{m}, \quad j = 1,2,..., p.$$

Theorem 2.1 Any chemical balance weighing design $\mathbf{X}$ is optimal if and only if $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p$.

In the literature, some methods of construction of the optimal chemical balance weighing design based on the incidence matrices of some known block designs are presented, see Ceranka and Katulska (1999), Ceranka and Graczyk (2004). This paper is a supplement to the construction given in Ceranka and Graczyk (2004) and presents the results of nonsingularity problem in the situation when the construction of the design matrix is based on the incidence matrices of the balanced bipartite weighing designs. Let us recall the definition of the balanced bipartite weighing design given in Swamy (1982).

A balanced bipartite weighing design there is an arrangement of v treatments into b blocks in such a way that 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, moreover each pair of treatments from different subblocks appears together in λ_1 blocks and each pair of treatments from the same subblock appears together in λ_2 blocks. The integers v, b, r, k_1, k_2, λ_1, λ_2 are called the parameters of the balanced bipartite weighing design and satisfy the following equalities

$$vr = bk, \quad b = \frac{\lambda_1 v(v-1)}{2k_1k_2}, \; \lambda_2 = \frac{\lambda_1[k_1(k_1-1)+k_2(k_2-1)]}{2k_1k_2}, \; r = \frac{\lambda_1 k(v-1)}{2k_1k_2}.$$

Let $\mathbf{N}^*$ be the incidence matrix of such design with elements equal to 1 or 0. Next, using $\mathbf{N}^*$ we construct the matrix $\mathbf{N}$ by replacing in each column k_1 elements equal +1 that corresponds to the elements belonging to the first subblock by –1. Hence, we consider the design matrix

$$\mathbf{X} = \mathbf{N}'. \tag{2.1}$$

Each column of $\mathbf{X}$ in (2.1) contains k_1 elements equal to –1, k_2 elements equal to 1 and $v - k_1 - k_2$ elements equal to 0.

From Swamy (1982), we have the following Lemma.

Lemma 2.1 Any chemical balance weighing design $\mathbf{X}$ of the form (2.1) is nonsingular if and only if

$$k_1 \neq k_2. \tag{2.2}$$

The construction of the optimum chemical balance weighing design of the form (2.1) for which the condition (2.2) is fulfilled is given in Ceranka, Katulska (1999). In the paper, we consider another case. Let us assume that for a given p and n, the design is singular, we can omit the problem of singularity by adding one more measurement operation. Then the design matrix is given by

$$\mathbf{X}^* = \begin{bmatrix} \mathbf{N}' \\ \mathbf{x}' \end{bmatrix}, \tag{2.3}$$

where $\mathbf{x} = \delta \mathbf{1}_v$, $\delta = 1$ or – 1.

Theorem 2.2 Any chemical balance weighing design $\mathbf{X}^*$ of the form (2.3) is nonsingular.

Proof. For the design matrix $\mathbf{X}^*$ given in (2.3), we get

$$\mathbf{X}^{*'}\mathbf{X}^* = (r - \lambda_2 + \lambda_1)\mathbf{I}_v + (\lambda_2 - \lambda_1 + 1)\mathbf{1}_v\mathbf{1}_v'. \tag{2.4}$$

Thus $\det(\mathbf{X}^{*'}\mathbf{X}^*) = (r - \lambda_2 + \lambda_1)^{v-1} \cdot [r + (v-1)(\lambda_2 - \lambda_1) + v]$. Taking into account the relations between the parameters of the balanced bipartite weighing design we obtain that $\det(\mathbf{X}^{*'}\mathbf{X}^*) = \lambda_1(v-1)(k_1 - k_2)^2 + 2vk_1k_2$ which is greater than zero. Hence the Theorem.

Theorem 2.3 Any chemical balance weighing design $\mathbf{X}^*$ of the form (2.3) is optimal if and only if $\lambda_1 = \lambda_2 + 1$.

Proof. For the design $\mathbf{X}^*$ in (2.3), considering (2.4), from the Theorem 2.1 we get that $\lambda_1 = \lambda_2 + 1$. Hence the thesis.

From the Theorem 2.1, we obtain $m = r + 1$ and $\mathrm{Var}(\hat{w}_j) = \frac{\sigma^2}{r+1}$.

Based on Ceranka and Graczyk (2002) we are able to formulate the following theorem.

Theorem 2.4 If the parameters of the balanced bipartite weighing design are equal to

(i) $v = 4s + 1$, $b = s(4s+1)$, $r = 4s$, $k_1 = k_2 = 2$, $\lambda_1 = 2$, $\lambda_2 = 1$,

(ii) $v = 4s$, $b = s(4s-1)$, $r = 4s - 1$, $k_1 = k_2 = 2$, $\lambda_1 = 2$, $\lambda_2 = 1$,

where $s = 1, 2, \ldots$, then any chemical balance weighing design $\mathbf{X}^*$ of the form (2.3) is optimal.

Proof. It is easy to check, that the parameters of the balanced bipartite weighing design (i) and (ii) satisfy the condition given in Theorem 2.3.

From Huang (1976) and Ceranka and Graczyk (2005) we receive the following theorem.

Theorem 2.5 If the parameters of the balanced bipartite weighing design are equal to $v = 2k_1$, $b = 2k_1 - 1$, $r = 2k_1 - 1$, k_1, $k_2 = k_1$, $\lambda_1 = k_1$, $\lambda_2 = k_1 - 1$, then any chemical balance weighing design $\mathbf{X}^*$ of the form (2.3) is optimal.

Proof. It is obvious, that the parameters of the balanced bipartite weighing design satisfy the condition $\lambda_1 = \lambda_2 + 1$ given in Theorem 2.3.

In addition, considering the paper of Ceranka and Graczyk (2004) we can formulate the theorem.

Theorem 2.6 If the parameters of the balanced bipartite weighing design are equal to

(i) $v = 4s$, $b = 4s - 1$, $r = 4s - 1$, $k_1 = 2s$, $k_2 = 2s$, $\lambda_1 = 2s$, $\lambda_2 = 2s - 1$,

(ii) $v = 4s$, $b = s(4s-1)$, $r = 4s - 1$, $k_1 = 2$, $k_2 = 2$, $\lambda_1 = 2$, $\lambda_2 = 1$,

(iii) $v = 4s + 1$, $b = s(4s+1)$, $r = 4s$, $k_1 = 2$, $k_2 = 2$, $\lambda_1 = 2$, $\lambda_2 = 1$, where $s = 1,2,\ldots$, then any chemical balance weighing design $\mathbf{X}^*$ in the form (2.3) is optimal.

Proof. Without any problem one can show, that the parameters of the balanced bipartite weighing design (i) – (iii) satisfy the condition given in Theorem 2.3.

3. Example

Let us consider an experiment in which we determine unknown measurements of 5 objects using 6 measurements operations. We consider the balanced bipartite weighing design with the parameters $v = 5$, $b = 5$, $r = 4$, $k_1 = 2$, $k_2 = 2$, $\lambda_1 = 2$, $\lambda_2 = 1$ given by the incidence matrix $\mathbf{N}^* = \begin{bmatrix} 1_1 & 1_2 & 1_1 & 1_2 & 0 \\ 1_1 & 1_1 & 1_2 & 0 & 1_2 \\ 1_2 & 1_1 & 0 & 1_2 & 1_1 \\ 1_2 & 0 & 1_1 & 1_1 & 1_2 \\ 0 & 1_2 & 1_2 & 1_1 & 1_1 \end{bmatrix}$, where 1_ξ denotes the object belonging to the ξth subblock, $\xi = 1,2$. Next, we obtain the matrix $\mathbf{N} = \begin{bmatrix} -1 & 1 & -1 & 1 & 0 \\ -1 & -1 & 1 & 0 & 1 \\ 1 & -1 & 0 & 1 & -1 \\ 1 & 0 & -1 & -1 & 1 \\ 0 & 1 & 1 & -1 & -1 \end{bmatrix}$. Now, we form the matrix $\mathbf{X} = \begin{bmatrix} -1 & -1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 & 1 \\ -1 & 1 & 0 & -1 & 1 \\ 1 & 0 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 \end{bmatrix}$ in (2.1) with $\det\left(\mathbf{X}'\mathbf{X}\right) = 0$. Instead of $\mathbf{X}$, we consider the design matrix $\mathbf{X}^{*} = \begin{bmatrix} -1 & -1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 & 1 \\ -1 & 1 & 0 & -1 & 1 \\ 1 & 0 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}$ defined in (2.3).

We have $\det\left(\mathbf{X}^{*'}\mathbf{X}^{*}\right) = 3125$. The design is nonsingular and optimal, moreover $\mathrm{Var}\left(\hat{w}_j\right) = \frac{\sigma^2}{5}$ for $j = 1,2,...,5$.

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UWAGI O OPTYMALNYCH CHEMICZNYCH UKŁADACH WAGOWYCH

Streszczenie

W pracy rozważa się osobliwe układy wagowe. Przedstawiona została konstrukcja układu nieosobliwego w oparciu o macierz układu osobliwego.

Słowa kluczowe: dwudzielny układ bloków, optymalny chemiczny układ wagowy

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