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OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS UNDER THE RESTRICTION ON WEIGHINGS

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Abstract

The paper deals with the problem of estimating individual weights of objects, using a chemical balance weighing design under the restriction on the number in which each object is weighed. A lower bound for the variance of each of the estimated weights from this chemical balance weighing design is obtained and a necessary and sufficient condition for this lower bound to be attained is given. The incidence matrix of ternary balanced block design is used to construct optimum chemical balance weighing design under the restriction on the number in which each object is weighed.

Keywords: chemical balance weighing design, ternary balanced block design.

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1. Introduction

In an actual experiment, when all the required observations are taken in accordance with the model, the observational equations are expressed in the matrix notation as

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \tag{1.1}$$

where $\mathbf{y}$ is an $n \times 1$ column vector of the observed random variables y_i, $i = 1, 2, \ldots, n$, $\mathbf{X} = (x_{ij})$, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, p$, $p \leq n$, is a known $n \times p$ matrix with x_{ij} as its (i, j)th element, $\mathbf{w}$ is a $p \times 1$ column vector of unknown parameters w_j, $j = 1, 2, \ldots, p$, and $\mathbf{e}$ is an $n \times 1$ column vector of unobserved random errors e_i, $i = 1, 2, \ldots, n$.

We shall assume for the present purpose that the distribution of the random vector $\mathbf{e}$ is such that $E(\mathbf{e}) = \mathbf{0}_n$ and $Var(\mathbf{e}) = E(\mathbf{ee}') = \sigma^2 \mathbf{I}_n$, where E stands for the mathematical expectation, $Var(\mathbf{e})$ stands for the variance – covariance matrix of the random vector $\mathbf{e}$, σ^2 is the variance of e_i, $i = 1, 2, \ldots, n$, $\mathbf{0}_n$ is the $n \times 1$ column vector with zero elements everywhere, $\mathbf{I}_n$ is the $n \times n$ identity matrix. From the form of matrix $Var(\mathbf{e})$ it is evident that the errors e_i, $i = 1, 2, \ldots, n$, are uncorrelated.

Matrix $\mathbf{X}$ is referred to as the design matrix. When elements x_{ij}, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, p$, of matrix $\mathbf{X}$ are $-1, 0, 1$, then the model (1.1) is called chemical balance design.

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

$$\mathbf{X}'\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{y}, \tag{1.2}$$

where $\hat{\mathbf{w}}$ is the vector of the weights estimated by the least squares method.

A chemical balance weighing design is said to be singular or nonsingular, depending on whether the matrix $\mathbf{X}'\mathbf{X}$ is singular or nonsingular, respectively. It is obvious the matrix $\mathbf{X}'\mathbf{X}$ is nonsingular if and only if the matrix $\mathbf{X}$ is of full column rank $(= p)$.

Now, if $\mathbf{X}'\mathbf{X}$ is nonsingular, the least squares estimates of $\mathbf{w}$ are given by

$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{1.3}$$

and the variance - covariance matrix of $\hat{\mathsf{w}}$ is

$$Var(\hat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}. \tag{1.4}$$

Various aspects of chemical balance weighing designs have been studied by Raghavarao (1971) and Banerjee (1975). Hotelling (1944) has shown that the minimum attainable variance for each of the estimated weights for a chemical balance weighing design is σ^2/n and proved the theorem that each of the variances of the estimated weights attains the minimum if and only if $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$. This design is said to be optimum chemical balance weighing design. In other words, matrix $\mathbf{X}$ of an optimum chemical balance weighing design has as elements only -1 and 1. In this case several methods of constructing optimum chemical balance weighing designs are available in the literature.

However, due to practical limitations, it may not be possible to weight all objects simultaneously in all the weights. The problem is to choose matrix $\mathbf{X}$ in such a manner that the variance factors are minimized. Then optimum chemical balance weighing design problem reduces to minimizing some functions of $Var\,(\hat{\mathbf{w}})$.

Some methods of constructing chemical balance weighing designs in which the estimated weights are uncorrelated in the case when the design matrix $\mathbf{X}$ has elements $-1, 0$ and 1 were given by Swamy (1982), Ceranka, Katulska and Mizera (1998) and Ceranka and Katulska (1999).

A study of weighing designs is supposed to be helpful in routine weighing operations to determine weights of objects. Moreover, the weighing designs are applicable to a great variety of problems of measurements, not only of weights, but of lengths, voltages and resistances, concentrations of chemicals in solutions, in fact any measurements such that the measure is the linear function of separate measures with the coefficient equal to $-1, 0, 1$.

In the present paper we study another method of constructing the design matrix $\mathbf{X}$ for an optimum chemical balance weighing design under the restriction on the number in which each object is weighed. In the next section, a lower bound for the variance of each of the estimated weights resulting from the chemical balance weighing design is obtained and a necessary and sufficient condition for this lower bound to be attained is given. The incidence matrix of ternary balanced block design has been used to construct some optimum chemical balance weighing design.

2. Variance limit of estimated weights

Let $\mathbf{X}$ be an $n \times p$ matrix of rank p and $\mathbf{c}$ denote any $p \times 1$ column vector. Then, from Section 1c.1 (ii) (b) given by Rao (1973), we have

Lemma 2.1. *For an $n \times p$ matrix $\mathbf{X}$ of rank p and a $p \times 1$ column vector $\mathbf{c}$, the inequality*

$$\mathbf{c}'\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{c} \geq \frac{\left(\mathbf{c}'\mathbf{c}\right)^2}{\mathbf{c}'\left(\mathbf{X}'\mathbf{X}\right)\mathbf{c}} \tag{2.1}$$

holds, with equality attained if and only if $\mathbf{c}$ *is an eigenvector of* $\mathbf{X}'\mathbf{X}$.

Let m_j be the number of times in which the jth object is weighed, $j = 1, 2, ..., p$.

Theorem 2.1. *For any nonsingular chemical balance weighing design given by matrix* $\mathbf{X}$*, the variance of* $\hat{w}_j$ *for a particular* j *such that* $1 \leq j \leq p$ *cannot be less than* σ^2/m*, where* $m = \max\limits_{j=1,2,\ldots,p} m_j$.

Proof. Let $\mathbf{c}_j, j = 1, 2, ..., p$, be the vector equal to the jth column of $\mathbf{I}_p$. Then it follows that

$$\hat{w}_j = \mathbf{c}_j'\hat{\mathbf{w}}$$

and

$$Var\left(\hat{w}_j\right) = \sigma^2 \mathbf{c}_j'\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{c}_j.$$

Since the matrix $\mathbf{X}$ is of full column rank, then from Lemma 2.1 we have

$$Var\left(\hat{w}_j\right) \geq \sigma^2 \frac{\left(\mathbf{c}_j'\mathbf{c}_j\right)^2}{\mathbf{c}_j'\left(\mathbf{X}'\mathbf{X}\right)\mathbf{c}_j} = \sigma^2 \frac{1}{\sum\limits_{i=1}^{n} x_{ij}^2} = \frac{\sigma^2}{m_j} \geq \frac{\sigma^2}{m} \tag{2.2}$$

because elements x_{ij} =-1, 1 or 0 only and number of elements equal to $-1, 1$ in the jth column of $\mathbf{X}$ is equal to m_j. Hence the theorem.

When $m = n$, Theorem 2.1 was originally proved by Hotelling (1944).

Now, we investigate the necessary and sufficient condition under which the minimum variance for each of the estimated weights is attained.

Theorem 2.2. *For any* $n \times p$ *matrix* $\mathbf{X}$*, in which columns maximum number of elements equal to* -1 *and* 1 *is equal to* m*, of a nonsingular chemical balance weighing design, each of the variances of the estimated weights attains the minimum if and only if*

$$\mathbf{X}'\mathbf{X} = m\mathbf{I}_p. \tag{2.3}$$

Proof. To prove the necessity part we observe that the equality in (2.2) holds for any j if and only if

$$\mathbf{X}'\mathbf{X}\mathbf{c}_j = m_j\mathbf{c}_j,$$

and

$$\mathbf{c}_j'\mathbf{X}'\mathbf{X}\mathbf{c}_j = m, \quad j = 1, 2, ..., p.$$

These conditions imply that $\mathbf{X}'\mathbf{X} = diag\{m_1, m_2, ..., m_p\}$ and $m_1 = m_2 = ... = m_p = m$. Therefore we have (2.3). The proof for the sufficiency part is obvious.

Definition 2.1. A nonsingular chemical balance weighing design is said to be optimum for the estimating individual weights of objects if the variances of their estimators attain the lower bound given by Theorem 2.1., i.e., if

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

In other words, an optimum design is given by $\mathbf{X}$ satisfying (2.3).

Theorem 2.3. *If the $n_i \times p$ design matrices $\mathbf{X}_i$ are the matrices of optimum chemical balance weighing designs, $i = 1, 2, ..., t$, then $\mathbf{X} = \left[\mathbf{X}_1' \vdots \mathbf{X}_2' \vdots \cdots \vdots \mathbf{X}_t'\right]'$ is the $\left(\sum_{i=1}^{t} n_i\right) \times p$ design matrix of an optimum chemical balance weighing design.*

Proof. It is obvious that

$$\mathbf{X}'\mathbf{X} = \left(\sum_{i=1}^{t} m_i\right)\mathbf{I}_p = m\mathbf{I}_p.$$

Theorem 2.4. *If the $n_i \times p$ design matrices $\mathbf{X}_i$ are the matrices of optimum chemical balance weighing design, $i = 1, 2$ and $\mathbf{X}_1'\mathbf{1}_{n_1} = \mathbf{0}_p$, then*

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{1}_{n_1} \\ \mathbf{X}_2 & \mathbf{0}_{n_2} \end{bmatrix} \tag{2.4}$$

is the $(n_1 + n_2) \times (p + 1)$ design matrix of an optimum chemical balance weighing design if and only if $m_1 + m_2 = n_1$, where $\mathbf{1}_{n_1}$ denotes the $n_1 \times 1$ column vector of ones.

Proof. For the design matrix $\mathbf{X}$ given by (2.4) we have

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{1}_{n_1} \\ \mathbf{1}_{n_1}'\mathbf{X}_1 & n_1 \end{bmatrix} = \begin{bmatrix} (m_1+m_2)\,\mathbf{I}_p & \mathbf{0}_p \\ \mathbf{0}_p' & n_1 \end{bmatrix} = m\mathbf{I}_{p+1},$$

because $\mathbf{X}_1'\mathbf{1}_{n_1} = \mathbf{0}_p$ and $\mathbf{X}_1, \mathbf{X}_2$ are the matrices of the optimum chemical balance weighing design and $m_1 + m_2 = n_1\,(= m)$. Hence the theorem.

In a particular case when $\mathbf{X}_1 = \mathbf{X}_2$, we have

Corollary 2.1. *If $\mathbf{X}_1$ is the $n_1 \times p$ matrix of the optimum chemical balance weighing design and $\mathbf{X}_1'\mathbf{1}_{n_1} = \mathbf{0}_p$, then*

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{1}_{n_1} \\ \mathbf{X}_1 & \mathbf{0}_{n_1} \end{bmatrix} \tag{2.5}$$

is the $2n_1 \times (p+1)$ design matrix of an optimum chemical balance weighing design if and only if $2m_1 = n_1$.

Theorem 2.5. *If $\mathbf{X}_i$ is the $n_i \times p$ matrix of the optimum chemical balance weighing design, $i = 1, 2$, and $\mathbf{X}_1'\mathbf{X}_1 = \mathbf{X}_2'\mathbf{X}_2$, $\mathbf{X}_1'\mathbf{1}_{n_1} = \mathbf{0}_p$, then*

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_1 & \mathbf{1}_{n_1} \\ \mathbf{X}_2 & -\mathbf{X}_2 & \mathbf{0}_{n_2} \end{bmatrix} \tag{2.6}$$

is the $(n_1 + n_2) \times (2p+1)$ design matrix of an optimum chemical balance weighing design if and only if $m_1 = m_2 = m$ and $2m = n_1$.

Proof. For the design matrix $\mathbf{X}$ given by (2.6) we have

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{X}_1 - \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{1}_{n_1} \\ \mathbf{X}_1'\mathbf{X}_1 - \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 & \mathbf{X}_1'\mathbf{1}_{n_1} \\ \mathbf{1}_{n_1}'\mathbf{X}_1 & \mathbf{1}_{n_1}'\mathbf{X}_1 & n_1 \end{bmatrix} = n_1\mathbf{I}_{p+1}.$$

In the next section, we will construct the optimum chemical balance weighing design based on ternary balanced block design.

3. Construction of the design matrix using ternary balanced block design

Let $\mathbf{N}$ be the incidence matrix of the ternary balanced block design with the parameters $v, b, r, k, \lambda, \rho_1, \rho_2$. Now we define the matrix $\mathbf{X}$ of a chemical balance weighing design as

$$\mathbf{X} = \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v'. \tag{3.1}$$

In this design we have $n = b$ and $p = v$. Thus, each column of $\mathbf{X}$ will contain ρ_2 elements equal to 1, $b-\rho_1-\rho_2$ elements equal to -1 and ρ_1 elements equal to 0. Clearly, such a design implies that each object is weighed $m = b - \rho_1$ times in the b weighing operations.

Lemma 3.1. *A design given by* $\mathbf{X}$ *of the form* (3.1) *is nonsingular if and only if* $v \neq k$.

Proof. For the design matrix $\mathbf{X}$ given by (3.1) we have

$$\mathbf{X}'\mathbf{X} = (r + 2\rho_2 - \lambda)\,\mathbf{I}_v + (b - 2r + \lambda)\,\mathbf{1}_v\mathbf{1}_v'. \tag{3.2}$$

It is easy to see that $det\,(\mathbf{X}'\mathbf{X}) = \frac{r}{k}\,(r + 2\rho_2 - \lambda)^{v-1}\,(v-k)^2$.

Evidently, $r + 2\rho_2 - \lambda$ is positive and then $det\,(\mathbf{X}'\mathbf{X}) = 0$ if and only if $v = k$. So, the lemma is proved.

Theorem 3.1. *A chemical balance weighing design with the matrix* $\mathbf{X}$ *given by* (3.1) *is optimal if and only if*

$$b = 2r - \lambda. \tag{3.3}$$

Proof. From the conditions (2.3) and (3.2) follows, that chemical balance weighing design is optimal if and only if $b-2r+\lambda=0$. Hence the theorem.

If the chemical balance weighing design given by matrix $\mathbf{X}$ of the form (3.1) is optimal, then

$$Var\,(\hat{w}_j)=\frac{\sigma^2}{m}=\frac{\sigma^2}{b-\rho_1}=\frac{\sigma^2}{r+2\rho_2-\lambda},\qquad j=1,2,...,p.$$

We have seen in Theorem 3.1 that if parameters of ternary balanced block design satisfy the condition (3.3), then a chemical balance weighing design with matrix $\mathbf{X}$ given by (3.1) is optimal. Under this condition we have formulated a theorem following from Billington and Robinson (1983) and Billington (1984).

Theorem 3.2. *The existence of a ternary balanced block designs with the parameters*

(i) $v=t, b=ut, r=u\,(t-2)\,, k=t-2, \lambda=u\,(t-4),\ \rho_1=u\,(t-4),$ $\rho_2=u,\ u=1,2,...,\ t=5,6,...,$ *except the case* $u=1$ *and* $t=5,$

(ii) $v=t, b=ut, r=u\,(t-3)\,, k=t-3, \lambda=u\,(t-6),\ \rho_1=u\,(t-9),$ $\rho_2=3u,\ u=1,2,...,\ t=10,11,...,$

(iii) $v=t, b=ut, r=u\,(t-4)\,, k=t-4, \lambda=u\,(t-8),\ \rho_1=u\,(t-16),$ $\rho_2=6u,\ u=1,2,...,\ t=17,18,...,$

(iv) $v=12t, b=4ut, r=u\,(4t-1)\,, k=3\,(4t-1)\,, \lambda=2u\,(2t-1),\ \rho_1=$ $u\,(4t-3),\ \rho_2=u,\ u=4,5,...,\ t=1,2,...,$

implies the existence of optimum chemical balance weighing design with matrix $\mathbf{X}$ *given by* (3.1).

Based on the Theorem 3.2 we present the list of all parameters combinations of the existing ternary balanced block designs under the restriction $r\leq 10$, those give optimum chemical balance weighing designs.

Table 1.

v	b	r	k	λ	ρ_1	ρ_2	m	v	b	r	k	λ	ρ_1	ρ_2	m
5	10	6	3	2	2	2	8	10	10	7	7	4	1	3	9
5	15	9	3	3	3	3	12	10	10	8	8	6	6	1	4
6	6	4	4	2	2	1	4	11	11	8	8	5	2	3	9
6	12	8	4	4	4	2	8	11	11	9	9	7	7	1	4
7	7	5	5	3	3	1	4	12	12	9	9	6	3	3	9
7	14	10	5	6	6	2	8	12	12	10	10	8	8	1	4
8	8	6	6	4	4	1	4	13	13	10	10	7	4	3	9
9	9	7	7	5	5	1	4								

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