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OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS CONSTRUCTED FROM THE INCIDENCE MATRICES OF THE TERNARY BALANCED BLOCK DESIGNS

Abstract. The paper studies the problem of estimation of the weights of p objects in n weighings using a chemical balance weighing design. $\mathbf{X} = (x_j)$ is an $n \times p$ matrix of a chemical balance weighing design and $x_{ij} = -1$, 1 or 0, if the j th object is kept on the right pan, left pan, or is not included in the particular weighing operation. This design is said to be optimum chemical balance weighing design when a lower bound for the variance of each of the estimated weights is obtained. A necessary and sufficient condition for this lower bound to be attained is given. The set of incidence matrices of ternary balanced block designs is used to construct the design matrix $\mathbf{X}$ of an optimum chemical balance weighing design under the restriction on the number in which each object is weighted.

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

1. INTRODUCTION

In a chemical balance weighing problem the results of n weighing operations are used to determine the individual weights of p light objects with a balance. Let $i = 1, 2, ..., n$, $j = 1, 2, ..., p$

$$x_{ij} = \begin{cases} 1, & \text{if the } j\text{th object is kept on the left pan in the } i\text{-th weighing,} \\ -1, & \text{if the } j\text{th object is kept on the right pan in the } i\text{-th weighing,} \\ 0, & \text{if the } j\text{th object is not weighed in the } i\text{-th weighing.} \end{cases}$$

An $n \times p$ matrix $\mathbf{X} = (x_{ij})$ is called the weighing design matrix. Let $\mathbf{w}$ be a column vector of true weights $w_1, w_2, ..., w_p$ and let $\mathbf{y}$ be a column vector

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of the readings $y_1, y_2, \ldots, y_n$. Then the vector of readings can be represented by the matrix equation

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

where $\mathbf{e}$ is a column vector of random errors between observed and expected readings. We assume that the random vector variable $\mathbf{e}$ is distributed with mean $\mathbf{O}_n$ and dispersion matrix $\sigma^2\mathbf{I}_n$, where $\mathbf{O}_n$ is $n \times 1$ vector with elements equal to 0 everywhere and $\mathbf{I}_n$ is the $n \times n$ identity matrix.

The least-squares estimates of true weights are estimated by $\hat{\mathbf{w}}$, where

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

When the weighing design matrix $\mathbf{X}$ is of full column rank we have

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

and

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

Various aspects of chemical balance weighing designs have been studied by D. Raghavarao (1971) and K. S. Banerjee (1975). H. Hotelling (1944) have showed 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.

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, 1 and 0 was given by M. N. Swamy (1982), B. Ceranka, K. Katulska and D. Mizera (1998) and B. Ceranka and K. Katulska (1999).

In the present paper we study another method of constructing the design matrix $\mathbf{X}$ for an optimum chemical balance weighing design, which has elements equal to –1, 1 and 0, under the restriction on the number in which each object is weighted. This method is based on the set of t incidence matrices of ternary balanced block designs.

2. VARIANCE LIMIT OF ESTIMATED WEIGHTS

Let $\mathbf{X}$ be an $n \times p$ matrix of rank p of a chemical balance weighing design and let m_j be the number of times in which j-th object is weighted, $j = 1, 2, ..., p$. B. Ceranka and M. Graczyk (2001) proved the following theorems:

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 $1 \leqslant j \leqslant p$ cannot be less than σ^2/m, where $m = \max_{j=1,2,...,p} (m_j)$.

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

$$\mathbf{X}'\mathbf{X} = m\mathbf{I}_p \tag{2.1}$$

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

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

In other words, an optimum design is given by $\mathbf{X}$ satisfying (2.1).

In the next sections we will present construction of matrix $\mathbf{X}$ of optimum chemical balance weighing design based on set of t incidence matrices of ternary balanced block designs.

3. TERNARY BALANCED BLOCK DESIGN

A ternary balanced block design is defined as me design consisting of b blocks, each of size k, chosen from a set of size v in such a way that each of the v elements occurs r times altogether and 0, 1 or 2 times in each block (2 appears at least one and each of the $\binom{v}{2}$ distinct pairs appears λ times). Any ternary balanced block design is regular, that is,

each element occurs alone in ρ_1 blocks and is repeated two times in ρ_2 blocks, where ρ_1 and ρ_2 are constant for the design. Let $\mathbf{N}$ be the incidence matrix of the ternary balanced block design. It is straightforward to verify that

$$vr = bk,$$
$$r = \rho_1 + 2\rho_2,$$
$$\lambda(v-1) = \rho_1(k-1) + 2\rho_2(k-2) = r(k-1) - 2\rho_2,$$
$$\mathbf{NN}' = (\rho_1 + 4\rho_2 - \lambda)\mathbf{I}_v + \lambda \mathbf{1}_v\mathbf{1}_v' = (r + 2\rho_2 - \lambda)\mathbf{I}_v + \lambda \mathbf{1}_v\mathbf{1}_v',$$

where $\mathbf{1}_v$ is $v \times 1$ vector with elements equal to 1 everywhere.

4. CONSTRUCTION

Let $\mathbf{N}_i^*$, $i = 1, 2, \ldots, t$ denote the incidence matrices of order $v \times b_i$ of ternary balanced block designs with parameters v, b_i, r_i, k_i, λ_i, ρ_{i1}, ρ_{2i}. From matrices $\mathbf{N}_i^*$ we obtain the matrices $\mathbf{N}_i = \mathbf{N}_i^* - \mathbf{1}_v\mathbf{1}_{b_i}'$, $i = 1, 2, \ldots, t$. Now we construct the matrix $\mathbf{X}$ of chemical balance weighing design in the form

$$\mathbf{X}' = [\mathbf{N}_1 \vdots \mathbf{N}_2 \vdots \cdots \vdots \mathbf{N}_t \vdots \mathbf{T}'] \tag{4.1}$$

where $\mathbf{T}' = \mathbf{k}_h\mathbf{1}_v'$ is matrix of order $h \times v$ $(h > 0)$, $\mathbf{k}_h$ is the column vector that has h_1 elements equal to 1 $(0 \leqslant h_1 \leqslant h)$ and $h - h_1$ elements equal to -1. If $h = 0$ then we take

$$\mathbf{X}' = [\mathbf{N}_1 \vdots \mathbf{N}_2 \vdots \cdots \vdots \mathbf{N}_t] \tag{4.2}$$

The matrix $\mathbf{X}$ given by (4.1) or (4.2) is design matrix of a chemical balance weighing design for $p = v$ objects in $n = \sum_{i=1}^{t} b_i + h$ weighings, where $h \geqslant 0$.

Theorem 4.1. The existence of t ternary balanced block designs with parameters v, b_i, r_i, k_i, λ_i, ρ_{1i}, ρ_{2i}, $i = 1, 2, \ldots, t$, satisfying

$$\sum_{i=1}^{t} b_i \leqslant \sum_{i=1}^{t} (2r_i - \lambda_i) \tag{4.3}$$

implies the existence of an optimum chemical balance weighing design for v objects in $\sum_{i=1}^{t} (2r - \lambda_t)$ weighings.

Proof. For the design matrix **X** given by (4. 1) we have

$$\mathbf{X}'\mathbf{X} = \left[\sum_{i=1}^{t}(\rho_{1i}+4\rho_{2i}+b_i-2r_i)-\alpha\right]\mathbf{I}_v+(\alpha+h)\mathbf{1}_v\mathbf{1}_v',$$

where $\alpha = \sum_{i=1}^{t} b_i - \sum_{i=1}^{t}(2r_i-\lambda_i)$. Now we assume that $\sum_{i=1}^{t} b_i = \sum_{i=1}^{t}(2r_t-\lambda_i)$. It means that $\alpha = 0$. Then

$$\mathbf{X}'\mathbf{X} = \left[\sum_{i=1}^{t}(\rho_{1i}+4\rho_{2i}+b_i-2r_i)\right]I_v+h\mathbf{1}_v\mathbf{1}_v'.$$

If in addition $h = 0$, then from Def. 2.1 the matrix **X** given by (4.2) is the design matrix of an optimum chemical balance weighing design.

Now, we assume that $\sum_{i=1}^{t} b_i < \sum_{i=1}^{t}(2r-\lambda_i)$ which means that $\alpha<0$. In such case we take $h=-\alpha$. In consequence the matrix

$$\mathbf{X}'\mathbf{X} = \left[\sum_{i=1}^{t}(\rho_{1i}+4\rho_{2i}+b_i-2r_i)+h\right]\mathbf{I}_v = \left[\sum_{i=1}^{t}(\rho_{1i}+4\rho_{2i}-\lambda_i)\right]\mathbf{I}_v.$$

Hence, from Def. 2.1, the matrix **X** given by (4.1) is the design matrix of an optimum chemical balance weighing design if $h=-\alpha$.

In particular case of $t=1$ we have obviously the following corollaries.

Corollary 4.1. The existence of a ternary balanced block design with parameters v, b, r, k, λ, ρ_1, ρ_2, satisfying $b \leqslant 2r-\lambda$, implies the existence of an optimum chemical balance weighing design for v objects in $2r-\lambda$ weighings.

Corollary 4.2. A chemical balance weighing design with **X** given by (4.2) is optimum if $\alpha = 0$

Corollary 4.3. A chemical balance weighing design with **X** given by (4.1) is optimum if $\alpha<0$ and $h=-\alpha$.

The condition $\alpha = 0$ implies $k_i \neq k_j$ for at least one pair (i, j), $i \neq j = 1, 2, \ldots, t$ or $k_1 = k_2 = \ldots = k_t = k \neq v$. Hence from Cor. 4.2 we have

Corollary 4.4. If a chemical balance weighing design with **X** given by (4.2) is optimum, then $k_i \neq k_j$ for at least one pair (i, j), $i = 1, 2, \ldots, t$ or $k_1 = k_2 = \ldots = k_t = k \neq v$.

If $k_1 = k_2 = \ldots = k_t = k = v$, then always $\alpha<0$. In this case we obtain two series of ternary balanced block designs with the parameters: the first: $v = k = 2a+1$, $b = r = 2a(p+1)+p+u$, $\lambda = 2a(p+1)+u-1$, $\rho_1 = p+u$,

$\rho_2 = a(p+1)$, where $a = 1, 2, ...,$ $p = 0, 1, ...,$ $u = 1, 2, ...,$ and the second: $v = k = 2a$, $b = r = \rho + 2u(2a-1)$, $\lambda = \rho + 4u(a-1)$, $\rho_1 = \rho$, $\rho_2 = (2a-1)u$, where $a = 2, 3, ...,$ $u = 1, 2, ...,$ $\rho = 1, 2, ...$

Corollary 4.5. If a ternary balanced block design with the parameters $v = k = 2a+1$, $b = r = 2a(p+1)+p+u$, $\lambda = 2a(p+1)+u-1$, $\rho_1 = p+u$, $\rho_2 = a(p+1)$ exist, where $a = 1, 2, ...,$ $p = 0, 1, ...,$ $u = 1, 2, ...,$ and $h = t(p+1)$ then a chemical balance weighing design for v objects in $n = t[(p+1)(2a+1)+p+u]$ weighing operations with matrix $\mathbf{X}$ given by (4.1) is optimum.

Corollary 4.6. If a ternary balanced block design with the parameters $v = k = 2a$, $b = r = p + 2u(2a-1)$, $\lambda = p + 4u(a-1)$, $\rho_1 = p$, $\rho_2 = (2a-1)u$ exist, where $a = 2, 3, ...,$ $u = 1, 2, ...,$ $p = 1, 2, ...,$ and $h = 2tu(a-1)$ then a chemical balance weighing design for v objects in $n = p + 2u[2a + 1t(a-1)]$ weighing operations with matrix $\mathbf{X}$ given by (4. 1) is optimum.

For example, an optimum chemical balanced weighing design for $v = 9$ objects and $n = 69$ weighing operations can be constructed from five ternary balanced block designs with parameters: $v = 9$, $b_1 = 9$, $r_1 = 9$, $k_1 = 9$, $\lambda_1 = 8$; $\rho_{11} = 1$, $\rho_{21} = 4$; $v = 9$, $b_2 = 10$, $r_2 = 10$, $k_2 = 9$, $\lambda_2 = 9$, $\rho_{12} = 2$, $\rho_{22} = 4$; $v = 9$, $b_3 = 11$, $r_3 = 11$, $k_3 = 9$, $\lambda_3 = 10$, $\rho_{13} = 3$, $\rho_{23} = 4$; $v = 9$, $b_4 = 12$, $r_4 = 12$, $k_4 = 9$, $\lambda_4 = 11$, $\rho_{14} = 4$, $\rho_{24} = 4$; $v = 9$, $b_5 = 27$, $r_5 = 15$, $k_5 = 5$, $\lambda_5 = 7$, $\rho_{15} = 11$, $\rho_{25} = 2$, respectively (see Th. 4. 1 and Cor. 4.2).

An optimum chemical balanced weighing design for $v = 9$ objects and $n = 39$ weighings can not be constructed from one ternary balanced block design, but from Th. 4.1 we can construct this design from three ternary balanced block designs with parameters: $v = 9$, $b_1 = 9$, $r_1 = 7$, $k_1 = 7$, $\lambda_1 = 5$, $\rho_{11} = 5$, $\rho_{21} = 1$; $v = 9$, $b_2 = 15$, $r_2 = 10$, $k_2 = 6$, $\lambda_2 = 6$, $\rho_{12} = 8$, $\rho_{22} = 1$; $v = 9$, $b_3 = 15$, $r_3 = 15$, $k_3 = 9$, $\lambda_3 = 14$, $\rho_{13} = 7$, $\rho_{23} = 4$, respectively.

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OPTYMALNY WAGOWY UKŁAD CHEMICZNY KONSTRUOWANY NA BAZIE MACIERZY POTRÓJNYCH BLOKÓW RÓWNOWAGI

W pracy podjęta została tematyka estymacji nieznanych miar p obiektów, gdy dysponujemy n operacjami pomiarowymi w modelu liniowym określanym jako chemiczny układ wagowy. W układzie tym pomiar jest liniową funkcją rzeczywistych miar obiektów o współczynnikach równych –1, 0 i 1. Chemiczny układ wagowy jest optymalny, gdy wariancje estymatorów wszystkich składowych wektora nieznanych miar obiektów są jednakowe i równe dolnemu ograniczeniu wariancji. Zatem podany został warunek konieczny i dostateczny, przy spełnieniu którego wariancja estymatorów osiąga dolne ograniczenie. Do konstrukcji macierzy optymalnego chemicznego układu wagowego wykorzystuje się zbiór t macierzy incydencji trójkowych zrównoważonych układów bloków.