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CONSTRUCTIONS OF OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS BASED ON BALANCED BLOCK DESIGNS

Abstract

The paper is studying the problem of estimation of the individual unknown measurements (weights) of p objects when we have at our disposal n measurement operations (weighings). In this problem we use the linear model called chemical balance weighing design under the restriction on the number times in which each object is measured. A lower bound for the variance of each of the estimated measurements and a necessary and sufficient conditions for this lower bound to be attained are given. The incidence matrices of balanced incomplete block designs and ternary balanced block designs are used to construct the design matrix **X** of optimum chemical balance weighing design.

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

I. INTRODUCTION

The results of n measurement (weighing) operations are used to determine the individual weights of p objects with a balance with two pans that is corrected for bias. The linear model for this experiment is given in the form

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \tag{1}$$

where $\mathbf{y}$ is $n \times 1$ random column vector of the observed measurements (weights), $\mathbf{X} = (x_{ij})$, $i = 1, 2, ..., n$, $j = 1, 2, ..., p$, is the $n \times p$ matrix of known

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elements with $x_{ij} = -1$, 1 or 0 if the j-th object is kept on the right pan, left pan or is not included in the particularly measurement operation (weighing), respectively, $\mathbf{w}$ is the $p \times 1$ column vector representing the unknown measurements (weights) of objects and $\mathbf{e}$ is the $n \times 1$ column vector of random errors between observed and expected readings such that $\mathrm{E}(\mathbf{e}) = 0_n$, and $\mathrm{E}(\mathbf{ee}') = \sigma^2\mathbf{I}_n$. By the other words, we assume that random errors are uncorrelated and they have the same variances. $\mathbf{0}_n$ is the $n \times 1$ vector with elements equal to 0 everywhere and $\mathbf{I}_n$ is the $n \times n$ identity matrix, E stands for expectation and $\mathbf{e}'$ is used for transpose of $\mathbf{e}$.

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

$$\mathbf{X}'\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}'\mathbf{y}, \tag{2}$$

where $\hat{\mathbf{w}}$ is the vector of the unknown measurements (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 that the matrix $\mathbf{X}'\mathbf{X}$ is nonsingular if and only if the design matrix $\mathbf{X}$ is of full column rank $(= p)$. Now, if $\mathbf{X}'\mathbf{X}$ is nonsingular, the least squares estimator of $\mathbf{w}$ is given by

$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{3}$$

and the variance – covariance matrix of $\hat{\mathbf{w}}$ is given by

$$\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}. \tag{4}$$

Various aspects of chemical balance weighing designs have been studied by Raghavarao (1971) and Banerjee (1975). 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 the other words, matrix $\mathbf{X}$ of an optimum chemical balance weighing design has as elements only –1 and 1. That means, in each measurement operation all objects are included. 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 **X** has elements –1, 1 and 0 was given by Swamy (1982), Ceranka et al. (1998) and Ceranka and Katulska (1999).

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

II. VARIANCE LIMIT OF ESTIMATED WEIGHTS

Let **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, $j = 1, 2, ..., p$. Ceranka and Graczyk (2001) proved the following theorems:

Theorem 1. For any nonsingular chemical balance weighing design given by matrix **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 $m = \max\limits_{j=1,2,...,p} (m_j)$.

Theorem 2. For any $n \times p$ matrix **X** of a nonsingular chemical balance weighing design, 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

$$\mathbf{X}'\mathbf{X} = m\mathbf{I}_p. \tag{5}$$

Definition 1. A nonsingular chemical balance weighing design is said to be optimal for the estimation individual weights of objects if the variances of their estimators attain the lower bound given by Theorem 1., i.e., if

$$\text{Var}(\hat{w}_j) = \frac{\sigma^2}{m}, \quad j = 1, 2, ..., p. \tag{6}$$

In the other words, the optimum design is given by the matrix **X** satisfying condition (5).

In the next sections we will present construction of the design matrix **X** of optimum chemical balance weighing design based on incidence matrices of balanced incomplete block designs and ternary balanced block designs.

III. BALANCED BLOCK DESIGN

A balanced incomplete block design there is an arrangement of v treatments into b blocks, each of size k, in such a way, that each treatment occurs at most ones in each block, occurs in exactly r blocks and every pair of treatments occurs together in exactly λ blocks. The integers v, b, r, k, λ are called the parameters of the balanced incomplete block design. Let $\mathbf{N}$ be the incidence matrix of balanced incomplete block design. It is straightforward to verify that

$$vr = bk,$$

$$\lambda(v-1) = r(k-1),$$

$$\mathbf{NN}' = (r-\lambda)\mathbf{I}_v + \lambda\mathbf{1}_v\mathbf{1}_v',$$

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

A ternary balanced block design is defined as the 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 ones) 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. The parameters are not all independent and they are related by the following identities

$$vr = bk,$$

$$r = \rho_1 + 2\rho_2,$$

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

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

IV. CONSTRUCTION OF THE DESIGN MATRIX

Let $\mathbf{N}_1$ be the incidence matrix of balanced incomplete block design with the parameters v, b_1, r_1, k_1, λ_1 and $\mathbf{N}_2$ be the incidence matrix of ternary balanced block design with the parameters v, b_2, r_2, k_2, λ_2, ρ_{12},

ρ_{22}. The matrix $\mathbf{X}$ of a chemical balance weighing design we define in the following form

$$\mathbf{X} = \begin{bmatrix} 2 \cdot \mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' \\ \mathbf{N}_2' - \mathbf{1}_{b_2}\mathbf{1}_v' \end{bmatrix}. \tag{7}$$

Thus each column of $\mathbf{X}$ contains $b_1 - r_1 + b_2 - \rho_{12} - \rho_{22}$ elements equal –1, $r_1 + \rho_{22}$ elements equal 1 and ρ_{12} elements equal 0. In this design each of the $p = v$ objects is measured $m = b_1 + b_2 - \rho_{12}$ times in $n = b_1 + b_2$ weighing operations.

Lemma 1. The chemical balance weighing design with the design matrix $\mathbf{X}$ given in the form (7) is nonsingular if and only if

$$2k_1 \neq k_2 \tag{8}$$

or

$$2k_1 = k_2 \neq v. \tag{9}$$

Proof. For the design matrix $\mathbf{X}$ given by (7) we have

$$\mathbf{X}'\mathbf{X} = [4(r_1 - \lambda_1) + r_2 + 2\rho_{22} - \lambda_2]\mathbf{I}_v + [b_1 - 4(r_1 - \lambda_1) + b_2 + \lambda_2 - 2r_2]\mathbf{1}_v\mathbf{1}_v' \tag{10}$$

It is easy to calculate that the determinant (10) is equal

$$\det(\mathbf{X}'\mathbf{X}) = [4(r_1 - \lambda_1) + r_2 + 2\rho_{22} - \lambda_2]^{v-1} \cdot \\ \cdot \frac{1}{k_1 k_2}[v^2(r_1 k_2 + r_2 k_1) - 2vk_1 k_2(2r_1 + r_2) + k_1 k_2(4r_1 k_1 + r_2 k_2)]. \tag{11}$$

Evidently $4(r_1 - \lambda_1) + r_2 + 2\rho_{22} - \lambda_2$ is positive and hence $\det(\mathbf{X}'\mathbf{X})$ is positive if and only if $2k_1 \neq k_2$ or $2k_1 = k_2 \neq v$. So, the lemma is proved.

Theorem 3. The nonsingular chemical balance weighing design with matrix $\mathbf{X}$ given by (7) is optimal if and only if

$$b_1 - 4(r_1 - \lambda_1) + (b_2 + \lambda_2 - 2r_2) = 0. \tag{12}$$

Proof. From the conditions (5) and (10) it follows that a chemical balance weighing design is optimal if and only if the condition (12) holds. Hence the theorem.

If the chemical balance weighing design with the design matrix **X** given by (7) is optimal then

$$\mathrm{Var}(\hat{w}_j) = \frac{\sigma^2}{b_1 + b_2 - \rho_{12}}, \quad j = 1, 2, ..., p. \tag{13}$$

In particular the equality (12) is true when $b_1 = 4(r_1 - \lambda_1)$ and $b_2 = 2r_2 - \lambda_2$.

Corollary 1. If the conditions

$$b_1 = 4(r_1 - \lambda_1) \tag{14}$$

and

$$b_2 = 2r_2 - \lambda_2 \tag{15}$$

are true then a nonsingular chemical balance weighing design with the design matrix **X** given by (7) is optimal.

The balanced incomplete block designs for which the condition (14) holds belong to the family *A* (Raghavarao, 1971: 69). The series of ternary balanced block designs for which the condition (15) is true was given by Billington and Robinson (1983).

Corollary 2. A chemical balance weighing design with the design matrix **X** given by (7) based on balanced incomplete block designs for which the condition (14) holds and ternary balanced block designs for which the condition (15) holds for the same number of treatments is optimal.

We have seen in the Theorem 3 that if parameters of balanced incomplete block designs satisfied the condition $b_1 - 4(r_1 - \lambda_1) = \alpha$ and parameters of ternary balanced block designs satisfied the condition $b_2 - 2r_2 + \lambda_2 = -\alpha$, $\alpha \neq 0$, then a chemical balance weighing design with the design matrix **X** given by (7) is optimal. For $\alpha = -2, -1, 1, 2$ we have

Corollary 3. A chemical balance weighing design with the design matrix **X** given by (7) based on the incidence matrices of balanced incomplete block designs and ternary balanced block designs with parameters

(i) $v = 5,\ b_1 = 10,\ r_1 = 4,\ k_1 = 2,\ \lambda_1 = 1$ and $v = 5,\ b_2 = 5(s+4),\ r_2 = 3(s+4),\ k_2 = 3,\ \lambda_2 = s+6,\ \rho_{12} = s+12,\ \rho_{22} = s,\ s = 1, 2, ...,$

(ii) $v = 7,\ b_1 = 42,\ r_1 = 12,\ k_1 = 2,\ \lambda_1 = 2$ and $v = 7,\ b_2 = s+13,\ r_2 = s+13,\ k_2 = 7,\ \lambda_2 = s+11,\ \rho_{12} = s+1,\ \rho_{22} = 6,\ s = 1, 2, ...,$

(iii) $v = 11,\ b_1 = 11,\ r_1 = 5,\ k_1 = 5,\ \lambda_1 = 2$ and $v = 11,\ b_2 = 11,\ r_2 = 7,\ k_2 = 7,\ \lambda_2 = 4,\ \rho_{12} = 5,\ \rho_{22} = 1,$

(iv) $v = 12,\ b_1 = 33,\ r_1 = 11,\ k_1 = 4,\ \lambda_1 = 3$ and $v = 12,\ b_2 = 18,\ r_2 = 15,\ k_2 = 10,\ \lambda_2 = 11,\ \rho_{12} = 1,\ \rho_{22} = 7,$

(v) $v = 15,\ b_1 = 15,\ r_1 = 7,\ k_1 = 7,\ \lambda_1 = 3$ and $v = 15,\ b_2 = 3(s+4)$, $r_2 = 2(s+4),\ k_2 = 10,\ \lambda_2 = s+5,\ \rho_{12} = 6-2s,\ \rho_{22} = 2s+1,\ s = 1, 2$ is optimal.

In a special case, when $r_1 = \lambda_1$ then condition (12) is of the form

$$b_1 + b_2 + \lambda_2 - 2r_2 = 0. \tag{16}$$

Corollary 4. The existence of ternary balanced block designs with the parameters $v,\ b_2,\ r_2,\ k_2,\ \lambda_2,\ \rho_{12},\ \rho_{22}$ for which $b_2 < 2r_2 - \lambda_2$ implies the existence of optimum chemical balance weighing design with

$$\mathbf{X} = \begin{bmatrix} \mathbf{1}_{b_1}\mathbf{1}'_v \\ \mathbf{N}'_2 - \mathbf{1}_{b_2}\mathbf{1}'_v \end{bmatrix}, \tag{17}$$

where $b_1 = 2r_2 - \lambda_2 - b_2$.

Corollary 5. The chemical balance weighing design with the design matrix $\mathbf{X}$ given by (17) based on ternary balanced block designs with parameters

(i) $v = 2s+1,\ b_2 = 4s+u+1,\ r_2 = 4s+u+1,\ k_2 = 2s+1,\ \lambda_2 = 4s+u-1$, $\rho_{12} = u+1,\ \rho_{22} = 2s,\ s = 2, 3, \ldots,\ u = 1, 2, \ldots$,

(ii) $v = 2s,\ b_2 = 4s+u-2,\ r_2 = 4s+u-2,\ k_2 = 2s,\ \lambda_2 = 4s+u-4$, $\rho_{12} = u,\ \rho_{22} = 2s-1,\ s = 2, 3, \ldots,\ u = 1, 2, \ldots$

is optimal, where $b_1 = 2$.

Corollary 6. A chemical balance weighing design with the design matrix $\mathbf{X}$ given by (17) based on ternary balanced block designs with parameters

(i) $v = 5,\ b_2 = 5(s+1),\ r_2 = 4(s+1),\ k_2 = 4,\ \lambda_2 = 3s+2,\ \rho_{12} = 4s$, $\rho_{22} = 2,\ s = 1, 2, \ldots$,

(ii) $v = 12,\ b_2 = 18,\ r_2 = 15,\ k_2 = 10,\ \lambda_2 = 11,\ \rho_{12} = 1,\ \rho_{22} = 7$,

(iii) $v = s,\ b_2 = s+u-1,\ r_2 = s+u-1,\ k_2 = s,\ \lambda_2 = s+u-2,\ \rho_{12} = u$, $\rho_{22} = \frac{s-1}{2},\ s = 5, 9, 11, 15,\ u = 1, 2, \ldots$

is optimal, where $b_1 = 1$.

In a particular case, when $\lambda_2 = 2r_2$ then the condition (12) is of the form

$$b_1 - 4(r_1 - \lambda_1) + b_2 = 0. \tag{18}$$

Corollary 7. The existence of balanced incomplete block designs with the parameters $v,\ b_1,\ r_1,\ k_1,\ \lambda_1$ for which $b_1 < 4(r_1 - \lambda_1)$ implies the existence of optimum chemical balance weighing design with

$$\mathbf{X} = \begin{bmatrix} 2 \cdot \mathbf{N}_1' - \mathbf{1}_{b_1} \mathbf{1}_v' \\ \mathbf{1}_{b_2} \mathbf{1}_v' \end{bmatrix}, \tag{19}$$

where $b_2 = 4(r_1 - \lambda_1) - b_1$.

Corollary 8. A chemical balance weighing design with the design matrix $\mathbf{X}$ given by (19) based on balanced incomplete block designs with parameters

(i) $v = 4s + 1$, $b_1 = 2(4s + 1)$, $r_1 = 4s$, $k_1 = 2s$, $\lambda_1 = 2s - 1$, $s = 1, 2, ..., (4s + 1)$ is primer or primer power,

(ii) $v = 4(s + 1)$, $b_1 = 2(4s + 3)$, $r_1 = 4s + 3$, $k_1 = 2(s + 1)$, $\lambda_1 = 2s + 1$, $s = 1, 2, ...$

is optimal, where $b_2 = 2$.

Corollary 9. A chemical balance weighing design with the design matrix $\mathbf{X}$ given by (19) based on balanced incomplete block designs with parameters

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

(ii) $v = 4s + 3$, $b_1 = 4s + 3$, $r_1 = 2s + 1$, $k_1 = 2s + 1$, $\lambda_1 = s$, $s = 1, 2, ..., (4s + 3)$ is primer or primer power,

(iii) $v = 8s + 7$, $b_1 = 8s + 7$, $r_1 = 4s + 3$, $k_1 = 4s + 3$, $\lambda_1 = 2s + 1$, $s = 1, 2, ...,$

is optimal, where $b_2 = 1$.

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Streszczenie

W pracy omówiona została tematyka estymacji nieznanych miar (wag) p obiektów w sytuacji, gdy dysponujemy n operacjami pomiarowymi. Zastosowany model określany jest mianem chemicznego układu wagowego, przy czym ograniczona jest liczba pomiarów poszczególnych obiektów. Zostało podane dolne ograniczenie wariancji każdej składowej estymatora wektora nieznanych miar obiektów oraz warunki konieczne i dostateczne, przy spełnieniu których wariancje estymatorów osiągną to dolne ograniczenie. Do konstrukcji macierzy optymalnego chemicznego układu wagowego zostały wykorzystane macierze incydencji układów zrównoważonych o blokach niekompletnych oraz trójkowych zrównoważonych układów bloków.