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Some Remarks about Optimum Chemical Balance Weighing Design for $p = v + 1$ Objects

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Abstract

The problem of the estimation of unknown weights of $p = v + 1$ objects in the model of the chemical balance weighing design under the assumption that the measurement errors are uncorrelated and they have different variances is considered. The existence conditions determining the optimum design are presented.

1 Introduction

We consider the linear model

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

which describe how to determine unknown measurements of p objects using n weighing operations according to the design matrix $\mathbf{X} = (x_{ij})$, $x_{ij} = -1,\ 0,\ 1$, $i = 1, 2, ..., n,\ j = 1, 2, ..., p$. For each i, the result of experiment y_i is linear combination of unknown measurements of w_j with factors equal to x_{ij}. Each object is weighed at most m times. In the model (1.1) $\mathbf{y}$ is a $n \times 1$ random vector of the observed weights, and $\mathbf{w}$ is a $p \times 1$ vector representing unknown weights of objects. If we have at our disposal two measurements installations then we assume that there are no systematic errors and the errors are uncorrelated and have different variances, i.e., for the $n \times 1$ random vector of errors $\mathbf{e}$ we have $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and $\mathrm{E}(\mathbf{e}\mathbf{e}') = \sigma^2\mathbf{G}$, where $\mathbf{0}_n$ is the $n \times 1$ column vector of zeros, $\mathbf{G}$ is an $n \times n$ positive definite diagonal matrix of known elements

$$\mathbf{G} = \begin{bmatrix} \frac{1}{a}\mathbf{I}_{b_1} & \mathbf{0}_{b_1}\mathbf{0}'_{b_2} \\ \mathbf{0}_{b_2}\mathbf{0}'_{b_1} & \mathbf{I}_{b_2} \end{bmatrix} \tag{1.2}$$

$a > 0$ is known scalar, $n = b_1 + b_2$. For the estimation of unknown weights of objects, we use the weighed least squares method and we get

$$\hat{\mathbf{w}} = \left(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{G}^{-1}\mathbf{y}$$

and the dispersion matrix of $\hat{\mathbf{w}}$ is

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

provided $\mathbf{X}$ is full column rank, i.e., $\mathrm{r}(\mathbf{X}) = p$.

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2 The optimality criterion

The concept of optimality comes from statistical theory of weighing designs.The optimality criterions which deal with the weighing designs were presented in Wong and Masaro (1984), Shah and Sinha (1989), Pukelsheim (1993). For $\mathbf{G} = \mathbf{I}_n$ the optimality criterions for chemical designs were presented in Raghavarao (1971), and Banerjee (1975). For the case that the errors are correlated with equal variances, the conditions determining the existence of the optimum chemical balance weighing design were considered in Ceranka and Graczyk (2003b). They gave the lower bound of variance of each of the estimators and the construction methods of the optimal design.

Let us consider the design matrix of the chemical balance weighing design for $p = v + 1$ objects as

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0}_{b_1} \\ \mathbf{X}_2 & \mathbf{1}_{b_2} \end{bmatrix}. \tag{2.1}$$

Definition 1 *Nonsingular chemical balance weighing design with the design matrix* $\mathbf{X}$ *and with the dispertion matrix of errors* $\sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is given in (1.2), is optimal if the variance of each of the estimators attains the lower bound.*

Now, we can formulate the conditions determining the optimality criterion. From Ceranka and Graczyk (2003a), we have

Theorem 1 *Any chemical balance weighing design with the design matrix* $\mathbf{X}$ *in the form (2.1) and with the dispertion matrix of errors* $\sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is given in (1.2), is optimal if and only if*

(i) $a\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 = (am_1 + m_2)\mathbf{I}_p$,

(ii) $\mathbf{X}_2'\mathbf{1}_{b_2} = \mathbf{0}_p$ and

(iii) $am_1 + m_2 = b_2$.

We note that in the optimum chemical balance weighing design with the design matrix given by (2.1), for each of $p = v + 1$ objects, we have

$$\mathrm{Var}(\hat{w}_j) = \frac{\sigma^2}{am_1 + m_2} = \frac{\sigma^2}{b_2}.$$

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

3 Balanced designs

Now, we recall the definitions of a balanced incomplete block design given in Raghavarao (1971) and of a ternary balanced block design given in Billington (1984).

In a balanced incomplete block design we replace v treatments in b blocks, each of size k, in such a way, that each treatment occurs at most once 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. The incidence relation between the treatments and blocks is denoted by the matrix $\mathbf{N} = (n_{ij})$, known as the incidence matrix, where n_{ij} denotes the number of times the ith treatment occurs in the jth block, $\mathbf{N}\mathbf{1}_b = \mathbf{r},\ \mathbf{N}'\mathbf{1}_v = \mathbf{k}$. It is straightforward to verify that

$$vr = bk,$$
$$\lambda(v-1) = r(k-1),$$
$$\mathbf{N}\mathbf{N}' = (r-\lambda)\mathbf{I}_v + \lambda\mathbf{1}_v\mathbf{1}_v',$$

where $\mathbf{1}_v$ is the $v \times 1$ vector of units.

A ternary balanced block design is defined as the design consisting of b blocks, each of size k, chosen from a set of objects of size v, in such a way that each of the v treatments occurs r times altogether and 0, 1 or 2 times in each block, (2 treatments appear together at least once). Each of the distinct pairs of objects appears λ times. Any ternary balanced block design is regular, that is, each treatment 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. It is straightforward to verify that

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

4 The optimality designs

Let $\mathbf{N}_1$ be the incidence matrix of the balanced incomplete block design with the parameters $v,\ b_1,\ r_1,\ k_1,\ \lambda_1$, and, let $\mathbf{N}_2$ be the incidence matrix of the ternary balanced block design with the parameters $v,\ b_2,\ r_2,\ k_2,\ \lambda_2,\ \rho_{12},\ \rho_{22}$. From the matrices $\mathbf{N}_1$ and $\mathbf{N}_2$, we construct the design matrix $\mathbf{X}$ of the chemical balance weighing design in the form (2.1) for $\mathbf{X}_1 = 2\mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v'$ and $\mathbf{X}_2 = \mathbf{N}_2' - \mathbf{1}_{b_2}\mathbf{1}_v'$,

$$\mathbf{X} = \begin{bmatrix} 2\mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' & \mathbf{0}_{b_1} \\ \mathbf{N}_2' - \mathbf{1}_{b_2}\mathbf{1}_v' & \mathbf{1}_{b_2} \end{bmatrix}. \tag{4.1}$$

Lemma 1 *Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (4.1) is nonsingular.*

Theorem 2 *Any chemical balance weighing design with the design matrix* $\mathbf{X}$ *in the form (4.1) and with the dispersion matrix* $\sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is given in (1.2), is optimal if and only if the conditions*

(i) $r_2 = b_2$

(ii) $a = \frac{\rho_{12}}{b_1}$

(iii) $a\left[b_1 - 4(r_1 - \lambda_1)\right] + b_2 + \lambda_2 - 2r_2 = 0$

are simultaneously fulfilled.

Proof. For the design matrix $\mathbf{X}$ in (4.1) and $\mathbf{G}$ in (1.2) we have

$$\mathbf{X}'\mathbf{G}^{-1}\mathbf{X} = \begin{bmatrix} \mathbf{T} & (r_2 - b_2)\mathbf{1}_v \\ (r_2 - b_2)\mathbf{1}_v' & b_2 \end{bmatrix},$$

where $\mathbf{T} =$
$\left[4a\left(r_1 - \lambda_1\right) + r_2 - \lambda_2 + 2\rho_{22}\right]\mathbf{I}_v + \left[a\left(b_1 - 4(r_1 - \lambda_1)\right) + b_2 - 2r_2 + \lambda_2\right]\mathbf{1}_v\mathbf{1}_v'$.
Using the optimality conditions given in the Theorem 2 our result is proved.

Based on Raghavarao (1971), Billington and Robinson (1983), Ceranka and Graczyk (2004), we can formulate

Theorem 3 *Let* $a = 2$. *If the parameters of the balanced incomplete block design and the parameters of the ternary balanced block design are equal to one of*

(i) $v = 7,\ b_1 = 21,\ r_1 = 6,\ k_1 = 2,\ \lambda_1 = 1$ and $v = k_2 = 7,\ b_2 = r_2 = 54,\ \lambda_2 = 52,\ \rho_{12} = 42,\ \rho_{22} = 6$;

(ii) $v = 12,\ b_1 = 33,\ r_1 = 11,\ k_1 = 4,\ \lambda_1 = 3$ and $v = k_2 = 12,\ b_2 = r_2 = 88,\ \lambda_2 = 86,\ \rho_{12} = 66,\ \rho_{22} = 11$; or

(iii) $v = b_1 = 13,\ r_1 = k_1 = 4,\ \lambda_1 = 1$ and $v = k_2 = 13,\ b_2 = r_2 = 50,\ \lambda_2 = 48,\ \rho_{12} = 26,\ \rho_{22} = 12$,

then $\mathbf{X}$ *in the form (4.1) is the design matrix of the optimum chemical balance weighing design with the dispersion matrix of errors* $\sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is in (1.2).*

Proof. It is easy to check that the parameters of the balanced bipartite weighing design and the ternary balanced block design satisfy the conditions (i) - (iii) of Theorem 2.

Theorem 4 *Let* $a = \frac{1}{2}$. *If the parameters of the balanced incomplete block design are equal to* $v = 15,\ b_1 = 42,\ r_1 = 14,\ k_1 = 5,\ \lambda_1 = 4$ *and the parameters of the ternary balanced block design are equal to* $v = k_2 = 15,\ b_2 = r_2 = 35,\ \lambda_2 = 34,\ \rho_{12} =$

$21,\ \rho_{22} = 7$, *then* $\mathbf{X}$ *in the form (4.1) is the design matrix of the optimum chemical balance weighing design with the dispersion matrix of errors* $\sigma^2\mathbf{G}$ *where* $\mathbf{G}$ *is in (1.2).*

Let us consider the design matrix $\mathbf{X}$ of the chemical balance weighing design in the form (2.1) for $\mathbf{X}_1 = 2\mathbf{N}_1^{'} - \mathbf{1}_{b_1}\mathbf{1}_v^{'}$ and $\mathbf{X}_2 = \mathbf{N}_2^{'} - \mathbf{1}_{b_2}\mathbf{1}_v^{'}$. We have

$$\mathbf{X} = \begin{bmatrix} 2\mathbf{N}_1^{'} - \mathbf{1}_{b_1}\mathbf{1}_v^{'} & \mathbf{1}_{b_1} \\ \mathbf{N}_2^{'} - \mathbf{1}_{b_2}\mathbf{1}_v^{'} & \mathbf{0}_{b_2} \end{bmatrix}. \qquad (4.2)$$

Theorem 5 *Any chemical balance weighing design with the design matrix* $\mathbf{X}$ *in the form (4.2) and with the dispersion matrix* $\sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is given in (1.2), does not exist.*

Proof. For the design matrix $\mathbf{X}$ in (4.1) and $\mathbf{G}$ in (1.2), we have

$$\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X} = \begin{bmatrix} \mathbf{T} & (2ar_1 - b_1)\mathbf{1}_v \\ (r_2 - b_2)\mathbf{1}_v^{'} & ab_1 \end{bmatrix},$$

where $\mathbf{T} =$
$[4a\,(r_1 - \lambda_1) + r_2 - \lambda_2 + 2\rho_{22}]\,\mathbf{I}_v + [a\,(b_1 - 4(r_1 - \lambda_1)) + b_2 - 2r_2 + \lambda_2]\,\mathbf{1}_v\mathbf{1}_v^{'}$.
Using the optimality conditions given in the Theorem 1 and comparing diagonal elements of $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$, we obtain $b_2 = \rho_{12}$. Therefore, a ternary balanced block design with parameters $v,\ b_2,\ r_2,\ k_2,\ \lambda_2,\ \rho_{12} = b_2,\ \rho_{22}$ does not exist.

5 Example

We consider two measurements installations and let $a = \frac{1}{2}$ be the factor determining the relation between the variances of both of them. We present the construction of the design matrix $\mathbf{X}$ given in Theorem 3 (ii). Let $\mathbf{G} = \begin{bmatrix} \frac{1}{2}\mathbf{I}_{b_1} & \mathbf{0}_{b_1}\mathbf{0}_{b_2}^{'} \\ \mathbf{0}_{b_2}\mathbf{0}_{b_1}^{'} & \mathbf{I}_{b_2} \end{bmatrix}$, and let $\mathbf{N}_1$ be the incidence matrix of the balanced incomplete block design with the parameters $v = 12,\ b_1 = 33,\ r_1 = 11,\ k_1 = 4,\ \lambda_1 = 3$ and let $\mathbf{N}_2$ be the incidence matrix of the ternary balanced block design with the parameters $v = k_2 = 12,\ b_2 = r_2 = 88,\ \lambda_2 = 86,\ \rho_{12} = 66,\ \rho_{22} = 11$, where

$$\mathbf{N}_1 = \begin{bmatrix}
1\,1\,1\,1\ 1\,1\,1\,1\,1\,1\,1\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0 \\
1\,1\,1\,0\,0\,0\,0\,0\,0\,0\,0\,1\,1\,1\,1\,1\,1\,1\,1\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0 \\
0\,0\,0\,1\,1\,1\,0\,0\,0\,0\,0\,1\,1\,1\,0\,0\,0\,0\,0\,1\,1\,1\,1\,1\,0\,0\,0\,0\,0\,0\,0\,0\,0 \\
0\,1\,0\,0\,0\,0\,1\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0\,0\,0\,1\,1\,1\,0\,0\,1\,1\,1\,1\,0\,0\,0\,0\,0 \\
0\,0\,0\,1\,0\,0\,1\,1\,0\,0\,0\,1\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0\,0\,0\,1\,1\,0\,0\,1\,1\,1\,0\,0 \\
1\,0\,1\,0\,0\,0\,0\,0\,1\,0\,0\,0\,0\,0\,0\,1\,0\,0\,0\,1\,1\,0\,1\,0\,0\,0\,0\,0\,1\,1\,0\,1\,1 \\
0\,0\,0\,0\,0\,0\,1\,0\,0\,1\,1\,1\,0\,1\,0\,0\,1\,0\,0\,0\,0\,0\,1\,0\,1\,0\,1\,0\,0\,0\,0\,1\,1 \\
0\,0\,0\,0\,1\,0\,0\,0\,0\,1\,1\,0\,0\,0\,0\,1\,1\,1\,1\,1\,0\,1\,0\,0\,0\,0\,1\,0\,1\,0\,1\,0\,0 \\
0\,1\,0\,0\,0\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0\,0\,0\,1\,1\,0\,0\,0\,1\,1\,1\,1\,0\,0\,0\,0\,1\,1\,0 \\
0\,0\,0\,0\,0\,1\,0\,0\,1\,1\,0\,0\,1\,1\,1\,0\,1\,0\,0\,0\,0\,0\,0\,1\,0\,0\,1\,1\,1\,1\,0\,0\,0 \\
0\,0\,0\,1\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0\,1\,0\,1\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0\,1\,0\,0\,1\,1\,1 \\
0\,0\,1\,0\,0\,0\,0\,1\,0\,0\,1\,0\,0\,1\,0\,0\,0\,0\,1\,0\,0\,1\,0\,1\,0\,1\,0\,1\,0\,1\,0\,0\,1
\end{bmatrix}$$

and $\mathbf{N}_2 = \left[\begin{array}{ccc} \mathbf{N}^* & \vdots & \mathbf{1}_{12}\mathbf{1}_{66} \end{array} \right]$, where

$$\mathbf{N}^* = \begin{bmatrix} 2\,2\,2\,2\,2\,2\,2\,2\,2\,2\,2\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0 \\ 2\,2\,2\,2\,2\,0\,0\,0\,0\,0\,0\,2\,2\,2\,2\,2\,2\,0\,0\,0\,0\,0 \\ 2\,2\,0\,0\,0\,2\,2\,2\,0\,0\,0\,2\,2\,2\,0\,0\,0\,2\,2\,2\,0\,0 \\ 0\,0\,2\,2\,0\,2\,2\,0\,2\,0\,0\,2\,2\,0\,2\,0\,0\,2\,0\,0\,2\,2 \\ 2\,0\,2\,0\,0\,2\,0\,0\,0\,2\,2\,0\,0\,2\,2\,2\,0\,2\,2\,0\,2\,0 \\ 0\,0\,2\,0\,2\,0\,2\,2\,0\,2\,0\,2\,0\,2\,0\,0\,2\,0\,2\,0\,2\,2 \\ 0\,2\,0\,2\,0\,0\,2\,0\,0\,2\,2\,0\,0\,2\,2\,0\,2\,2\,0\,2\,0\,2 \\ 2\,0\,0\,0\,2\,0\,2\,0\,2\,0\,2\,0\,2\,0\,2\,0\,2\,0\,2\,2\,2\,0 \\ 0\,2\,0\,0\,2\,2\,0\,0\,2\,2\,0\,2\,0\,0\,2\,2\,0\,0\,2\,2\,0\,2 \\ 0\,2\,2\,0\,0\,0\,0\,2\,2\,0\,2\,0\,2\,0\,0\,2\,2\,2\,2\,0\,0\,2 \\ 0\,0\,0\,2\,2\,2\,0\,2\,0\,0\,2\,0\,2\,2\,0\,2\,0\,0\,0\,2\,2\,2 \\ 2\,0\,0\,2\,0\,0\,0\,2\,2\,2\,0\,2\,0\,0\,0\,2\,2\,2\,0\,2\,2\,0 \end{bmatrix}.$$

From the matrices $\mathbf{N}_1$ and $\mathbf{N}_2$, we construct the design matrix $\mathbf{X}$ of the chemical balance weighing design in the form (4) as

$$\mathbf{X} = \begin{bmatrix} \mathbf{T}_1 & \mathbf{0}_{33} \\ \mathbf{T}_2 & \mathbf{1}_{22} \\ \mathbf{T}_3 & \mathbf{1}_{66} \end{bmatrix},$$

where $\quad \mathbf{T}_1 = 2\mathbf{N}_1' - \mathbf{1}_{33}\mathbf{1}_{12}', \quad \mathbf{T}_2 = (\mathbf{N}_2^*)' - \mathbf{1}_{22}\mathbf{1}_{12}', \quad \mathbf{T}_3 = -\mathbf{1}_{66}\mathbf{1}_{12}'$.
In this design, we estimate measurements of 12 objects with $\mathrm{Var}\,(\hat{w}_j) = \frac{\sigma^2}{88}$ for $j = 1, 2, ..., 12$.

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