A C T A U N I V E R S I T A T I S L O D Z I E N S I S
FOLIA OECONOMICA 228, 2009

Małgorzata Graczyk *

OPTIMUM CHEMICAL BALANCE WEIGHING DESIGN FOR $p = v + 1$ OBJECTS BASED ON BALANCED BLOCK DESIGNS

Abstract. The paper we study the problem of estimation of individual (weights) measurements p objects using n measurements operations according to the model of the chemical balance weighing design. We assume that in each measurement not all object are included. We give conditions under which the existence of the optimum chemical balance weighing design for $p = v$ objects implies the existence of the optimum chemical balance weighing design for $p = v + 1$ objects are given. For construction the design matrix $\mathbf{X}$ of the optimum chemical balance weighing design for $p = v + 1$ objects we use the incidence matrices of the balanced incomplete block designs and the balanced bipartite weighing designs for v treatments.

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

I. INTRODUCTION

We consider the experiment in which using n measurement (weighing) operations we determine unknown weights of given number of p objects The problem comes from statistical theory of weighing designs. The results of experiment we can write as

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

where $\mathbf{y}$ is $n \times 1$ random column vector of the observed weights, $\mathbf{X} = (x_{ij}),\ i = 1,2,...,n,\ j = 1,2,...,p$, called a design matrix, is matrix of known elements x_{ij}. If in the ith weighing jth object is placed on the left pan of scale then $x_{ij} = -1$, if on the right pan then $x_{ij} = 1$ and $x_{ij} = 0$ if jth object is omitted in the ith weighing. $\mathbf{w}$ is $p \times 1$ column vector representing unknown weights

* Ph.D., Department of Mathematical and Statistical Methods, Agricultural University of Poznań.

of objects and $\mathbf{e}$ is an $n \times 1$ random column vector of errors we have $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and $\mathrm{E}(\mathbf{ee}') = \sigma^2 \mathbf{I}_n$, where $\mathbf{0}_n$ is an $n \times 1$ column vector of zeros, $\mathbf{I}_n$ is an $n \times n$ identity matrix, $\mathrm{E}(\cdot)$ stands for the expectation of $(\cdot)$ and $(\cdot)'$ is used for the transpose of $(\cdot)$. For the estimation of unknown weights of objects we used the least squares method and we get

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

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

$$\mathrm{V}(\hat{\mathbf{w}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1},$$

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

Various aspects of the chemical balance weighing designs have been studied in Raghavarao (1971), Banerjee (1975) and Shah and Sinha (1989). 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 that each of the variance of each estimator of unknown weights of objects attains minimum if and only if $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$. This design is called optimum chemical balance weighing design. In other words, $\mathbf{X}$ is the design matrix of the optimum chemical balance weighing design if and only if its elements are equal to –1 or 1, only. In this case several construction methods of the design matrix are available in the literature. Some methods of construction of the design matrix of the optimum chemical balance weighing design under the restriction on the number of objects placed on the pans are given by Swamy (1982), Ceranka and Katulska (1999), Ceranka and Graczyk (2001a).

In the present paper we generalize problem given by Hotelling. We assume that in each measurement operation not all objects are included. That means the elements of the design matrix $\mathbf{X}$ are equal to –1, 1 or 0. Under this assumption we present new method of construction of the optimum chemical balance weighing design. In this method from the incidence matrices of the balanced incomplete block designs and the balanced bipartite weighing designs for v treatments we form the design matrix of optimum design for $p = v + 1$ objects.

II. 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 equal to the number of times in which j th object is weighted, or respectively number of elements equal to -1 and 1 in j th column of $\mathbf{X}$, $j = 1, 2, ..., p$. Ceranka and Graczyk (2001b) showed that the minimum attainable variance for each of the estimated weights for a chemical balance weighing design is σ^2/m, i.e. $\mathrm{V}(\hat{w}_j) \geq \sigma^2/m$, $m = \max\{m_1, m_2, ..., m_p\}$.

Definition 1. Any chemical balance weighing design $\mathbf{X}$ is called optimal for the estimation of individual weights if $\mathrm{V}(\hat{w}_j) \geq \sigma^2/m$, $j = 1,2,...,p$.

Ceranka and Graczyk (2001b) proved the following theorem

Theorem 1. Any nonsingular chemical balance weighing design $\mathbf{X}$ is optimal if and only if

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

In particular case when $m = n$ the theorem was given in Hotelling (1944).

III. BALANCED BLOCK DESIGN

In this section we recall definitions of the balanced incomplete block design given in Raghavarao (1971) and the balanced bipartite weighing design given in Swamy (1982).

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

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

A balanced bipartite weighing design there is an arrangement of v treatments into b blocks such 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. Every pair of treatments from different subblocks appears together in λ_1 blocks and every 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. Let $\mathbf{N}^*$ be the incidence matrix of such a design. The parameters are not independent and they are related by the following identities

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

$$r = \frac{\lambda_1 k(v-1)}{2k_1k_2}, \quad \mathbf{N}^*\mathbf{N}^{*'} = (r-\lambda_1-\lambda_2)\mathbf{I}_v + (\lambda_1+\lambda_2)\mathbf{1}_v\mathbf{1}_v^{'}.$$

IV. CONSTRUCTION

Let $\mathbf{N}_1$ be the incidence matrix of the balanced incomplete block design with the parameters v, b_1, r_1, k_1, λ_1, $\mathbf{N}_2^*$ be the incidence matrix of the balanced bipartite weighing design with the parameters v, b_2, r_2, k_{12}, k_{22}, λ_{12}, λ_{22} $(k_{12} < k_{22})$ and $\mathbf{N}_3^*$ be the incidence matrix of the balanced bipartite weighing design with the parameters v, $b_3 = b_2$, $r_3 = r_2$, $k_{13} = k_{22}$, $k_{23} = k_{12}$, $\lambda_{13} = \lambda_{12}$, $\lambda_{23} = \lambda_{22}$. Now, for $s = 2,3$, the $\mathbf{N}_s$ can be obtained from $\mathbf{N}_s^*$ by replacing the k_{1s} elements equal to +1 of each column which correspond to the elements belonging to the first subblock by –1. Thus each column of $\mathbf{N}_s$ will contain k_{1s} elements equal to –1, k_{2s} elements equal to 1 and $v - k_{1s} - k_{2s}$ elements equal to 0. Now, we define the design matrix $\mathbf{X}$ of the chemical balance weighing design as

$$\mathbf{X} = \begin{bmatrix} 2\mathbf{N}_1^{'} - \mathbf{1}_{b_1}\mathbf{1}_v^{'} \\ \mathbf{N}_2^{'} \\ \mathbf{N}_3^{'} \end{bmatrix}. \tag{1}$$

In this design each of $p = v$ objects is weighted $m = b_1 + 2r_2$ times in $n = b_1 + 2b_2$ measurement operations.

It is easy to show that chemical balance weighing design $\mathbf{X}$ in (1) is nonsingular if and only if $v \neq 2k_1$ or $k_{12} \neq k_{22}$.

Theorem 2. Any nonsingular chemical balance weighing design with the design matrix $\mathbf{X}$ given in (1) is optimal if and only if

$$b_1 - 4(r_1 - \lambda_1) + 2(\lambda_{22} - \lambda_{12}) = 0\,. \tag{2}$$

Proof. For the design matrix $\mathbf{X}$ given in (1) we have

$$\mathbf{X}'\mathbf{X} = (4(r_1 - \lambda_1) + 2(r_2 - \lambda_{22} + \lambda_{12}))\mathbf{I}_v + (b_1 - 4(r_1 - \lambda_1) + 2(\lambda_{22} - \lambda_{12}))\mathbf{1}_v\mathbf{1}_v'\,.$$

The thesis of Theorem is a result derived from Theorem 1.

Now, let $\mathbf{X}$ given in (1) be the matrix the optimum chemical balance weighing design for $p = v$ objects. Based on this matrix we construct the design matrix $\mathbf{X}$ of the chemical balance weighing design for $p = v + 1$ objects in the form

$$\mathbf{X} = \begin{bmatrix} 2\mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' & \mathbf{0}_{b_1} \\ \mathbf{N}_2' & \mathbf{1}_{b_2} \\ \mathbf{N}_3' & \mathbf{1}_{b_2} \end{bmatrix}. \tag{3}$$

In this design each of $p = v + 1$ and $n = b_1 + 2b_2$.

Theorem 3. If $\mathbf{X}$ given in (1) is the design matrix of the optimum chemical balance weighing design then $\mathbf{X}$ given in (3) is the design matrix of the optimum chemical balance weighing design if and only if

$$b_1 = 2(b_2 - r_2)\,. \tag{4}$$

Proof. For the design matrix $\mathbf{X}$ given in (3) we have

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} (b_1 + 2r_2)\mathbf{I}_v & \mathbf{0}_v \\ \mathbf{0}_v' & 2b_2 \end{bmatrix}.$$

Theorem 2 implies (4).

The equality (2) is true when $b_1 - 4(r_1 - \lambda_1) = 2(\lambda_{22} - \lambda_{12}) = \alpha$, $\alpha = 0, \pm 1, \pm 2, \ldots$. Now we consider particular case $\alpha = 0$.

We have seen in Theorem 1 that if the parameters of the balanced incomplete block design and the balanced bipartite weighing design satisfy the condition (2) then the chemical balance weighing design with the design matrix $\mathbf{X}$ given in (1) is optimal. If the chemical balance weighing design is optimal then from Theorem 2 the design matrix $\mathbf{X}$ given in (3) is optimal if and only if the condition (4) is fulfilled. Under these conditions we have formulated Theorem following from papers of Raghavarao (1971) and Huang (1976).

Theorem 4. The existence of the balanced incomplete block design with the parameters

$$v = s^2,\ b_1 = \frac{s(s^2-1)(s^2-4)}{6},\ r_1 = \frac{(s-1)(s^2-1)(s^2-4)}{12},$$

$$k_1 = \frac{s(s-1)}{2},\ \lambda_1 = \frac{(s-2)(s^2-1)(s^2-4)}{24}$$

and the balanced bipartite weighing design with the parameters $v = s^2$, $b_2 = \frac{s^3(s^2-1)}{12}$, $r_2 = \frac{s(s^2-1)}{3}$, $k_{12} = 1$, $k_{22} = 3$, $\lambda_{12} = \lambda_{22} = \frac{s}{2}$, $s \geq 4$ is even number except the case $s \equiv 0 (\mathrm{mod}\, 6)$, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Proof. It is easy to see that the parameters of the balanced incomplete block design and the balanced bipartite weighing design given in Theorem satisfy the condition (2).

Theorem 5. The existence of the balanced incomplete block design with the parameters

$$v = s^2,\ b_1 = \frac{s(s^2-1)(s^2-4)}{3},\ r_1 = \frac{(s-1)(s^2-1)(s^2-4)}{6},$$

$$k_1 = \frac{s(s-1)}{2},\ \lambda_1 = \frac{(s-2)(s^2-1)(s^2-4)}{12}$$

and the balanced bipartite weighing design with the parameters $v = s^2$, $b_2 = \frac{s^3(s^2-1)}{6}$, $r_2 = \frac{2s(s^2-1)}{3}$, $k_{12} = 1$, $k_{22} = 3$, $\lambda_{12} = \lambda_{22} = s$, s is odd number except the case $s \equiv 3(\mathrm{mod}\, 6)$, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 6. The existence of the balanced incomplete block design with the parameters

$$v = s^2,\ b_1 = s(s^2-1)(s^2-4),\ r_1 = \frac{(s-1)(s^2-1)(s^2-4)}{2},$$

$$k_1 = \frac{s(s-1)}{2},\ \lambda_1 = \frac{(s-2)(s^2-1)(s^2-4)}{4}$$

and the balanced bipartite weighing design with the parameters $v = s^2$, $b_2 = \frac{s^3(s^2-1)}{4}$, $r_2 = s(s^2-1)$, $k_{12} = 1$, $k_{22} = 3$, $\lambda_{12} = \lambda_{22} = \frac{3s}{2}$, $s \geq 4$ is even number, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 7. The existence of the balanced incomplete block design with the parameters

$$v = s^2,\ b_1 = s(s^2-1)(s^2-4),\ r_1 = \frac{(s-1)(s^2-1)(s^2-4)}{2},$$

$$v = s^2,\ b_1 = s(s^2-1)(s^2-4),\ r_1 = \frac{(s-1)(s^2-1)(s^2-4)}{2},$$

and the balanced bipartite weighing design with the parameters $v = s^2$, $b_2 = \frac{s^3(s^2-1)}{2}$, $r_2 = 2s(s^2-1)$, $k_{12} = 1$, $k_{22} = 3$, $\lambda_{12} = \lambda_{22} = 3s$, s is odd number, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 8. The existence of the balanced incomplete block design with the parameters

$$v = s^2,\ b_1 = \frac{2s(s^2-1)(s^2-9)}{9},\ r_1 = \frac{(s-1)(s^2-1)(s^2-9)}{9},$$

$$v=s^2,\ b_1=\frac{2s\left(s^2-1\right)\left(s^2-9\right)}{9},\ r_1=\frac{(s-1)\left(s^2-1\right)\left(s^2-9\right)}{9},$$

and the balanced bipartite weighing design with the parameters $v=s^2$, $b_2=\frac{s^3\left(s^2-1\right)}{9}$, $r_2=s\left(s^2-1\right)$, $k_{12}=3$, $k_{22}=6$, $\lambda_{12}=\lambda_{22}=4s$, $s\geq 6$ is even number, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 9. The existence of the balanced incomplete block design with the parameters

$$v=s^2,\ b_1=\frac{s\left(s^2-1\right)\left(s^2-9\right)}{3},\ r_1=\frac{(s-1)\left(s^2-1\right)\left(s^2-9\right)}{6},$$

$$k_1=\frac{s(s-1)}{2},\ \lambda_1=\frac{(s-2)\left(s^2-1\right)\left(s^2-9\right)}{24}$$

and the balanced bipartite weighing design with the parameters $v=s^2$, $b_2=\frac{s^3\left(s^2-1\right)}{12}$, $r_2=\frac{3s\left(s^2-1\right)}{4}$, $k_{12}=3$, $k_{22}=6$, $\lambda_{12}=\lambda_{22}=3s$, $s\geq 5$ is odd number, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Now we give the parameters of the balanced incomplete block design and the balanced bipartite weighing design for which the condition (2) is true for $\alpha\neq 0$.

Theorem 10. The existence of the balanced incomplete block design with the parameters $v=4s+1$, $b_1=2(4s+1)$, $r_1=4s$, $k_1=2s$, $\lambda_1=2s-1$ and the balanced bipartite weighing design with the parameters

(i) $v=4s+1$, $b_2=s(4s+1)$, $r_2=5s$, $k_{12}=1$, $k_{22}=4$, $\lambda_{12}=2$, $\lambda_{22}=3$ or

(ii) $v=4s+1$, $b_2=2s(4s+1)$, $r_2=14s$, $k_{12}=2$, $k_{22}=5$, $\lambda_{12}=10$ $\lambda_{22}=11$,

where $4s+1$ is a prime or a prime power, $s=1,2,\ldots$, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 11. The existence of the balanced incomplete block design with the parameters $v=10s+1$, $b_1=2(10s+1)$, $r_1=10s$, $k_1=5s$, $\lambda_1=5s-1$ and the balanced bipartite weighing design with the parameters $v=10s+1$, $b_2=s(10s+1)$,

$r_2 = 6s$, $k_{12} = 1$, $k_{22} = 5$, $\lambda_{12} = 1$ $\lambda_{22} = 2$, where $10s + 1$ is a prime or a prime power, $s = 1,2,\ldots$, implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 12. The existence of the balanced incomplete block design with the parameters $v = 7$, $b_1 = 42$, $r_1 = 12$, $k_1 = 2$, $\lambda_1 = 2$ and the balanced bipartite weighing design with the parameters

(i) $v = 7$, $b_2 = 21$, $r_2 = 9$, $k_{12} = 1$, $k_{22} = 2$, $\lambda_{12} = 2$, $\lambda_{22} = 1$ or

(ii) $v = 7$, $b_2 = 21$, $r_2 = 18$, $k_{12} = 2$, $k_{22} = 4$, $\lambda_{12} = 8$, $\lambda_{22} = 7$

implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 13. The existence of the balanced incomplete block design with the parameters $v = 10$, $b_1 = 30$, $r_1 = 9$, $k_1 = 3$, $\lambda_1 = 2$ and the balanced bipartite weighing design with the parameters $v = 10$, $b_2 = 45$, $r_2 = 27$, $k_{12} = 2$, $k_{22} = 4$, $\lambda_{12} = 8$, $\lambda_{22} = 7$ implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 14. The existence of the balanced incomplete block design with the parameters $v = 13$, $b_1 = 26$, $r_1 = 8$, $k_1 = 4$, $\lambda_1 = 2$ and the balanced bipartite weighing design with the parameters

(i) $v = 13$, $b_2 = 78$, $r_2 = 18$, $k_{12} = 1$, $k_{22} = 2$, $\lambda_{12} = 2$, $\lambda_{22} = 1$,

(ii) $v = 13$, $b_2 = 39$, $r_2 = 12$, $k_{12} = 2$, $k_{22} = 2$, $\lambda_{12} = 2$, $\lambda_{22} = 1$,

(iii) $v = 13$, $b_2 = 39$, $r_2 = 15$, $k_{12} = 2$, $k_{22} = 3$, $\lambda_{12} = 3$, $\lambda_{22} = 2$ or

(iv) $v = 13$, $b_2 = 78$, $r_2 = 36$, $k_{12} = 2$, $k_{22} = 4$, $\lambda_{12} = 8$, $\lambda_{22} = 7$

implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

Theorem 15. The existence of the balanced incomplete block design with the parameters $v = 15$, $b_1 = 42$, $r_1 = 14$, $k_1 = 5$, $\lambda_1 = 4$ and the balanced bipartite weighing design with the parameters

(i) $v = 15$, $b_2 = 105$, $r_2 = 21$, $k_{12} = 1$, $k_{22} = 2$, $\lambda_{12} = 2$, $\lambda_{22} = 1$ or

(ii) $v = 15$, $b_2 = 105$, $r_2 = 42$, $k_{12} = 2$, $k_{22} = 4$, $\lambda_{12} = 8$, $\lambda_{22} = 7$

implies the existence of the optimum chemical balance weighing design with the design matrix $\mathbf{X}$ given in (3).

REFERENCES

Banerjee, K.S. (1975), *Weighing designs for chemistry, medicine, economics, operations research, statistics*. Marcel Dekker Inc., New York.

Ceranka, B., Graczyk, M. (2001a), "Chemical balance weighing designs under the restriction on the number of weighings." Colloquium Biometryczne **31**, 39–45.

Ceranka B., Graczyk M., (2001b), "Optimum chemical balance weighing designs under the restriction of weighings." Discussiones Mathematicae – Probability and Statistics **21**, 111–120.

Ceranka, B., Katulska, K. (1999), "Chemical balance weighing design under the restriction on number of objects placed on the pans." Tatra Mt. Math. Publ. **17**, 141–148.

Huang, Ch. (1976), "Balanced bipartite block designs." *Journal of Combinatorial Theory* (**A**) **21**, 20–34.

Hotelling, H. (1944), "Some improvements in weighing designs and other experimental techniques." *Ann. Math. Stat.* **15**, 297–305.

Raghavarao, D. (1971), *Constructions and Combinatorial Problems in designs of Experiments*. John Wiley Inc., New York.

Shah, K.R., Sinha, B.K. (1989), *Theory of optimal designs*. Springer-Verlag, Berlin, Heidelberg.

Swamy, M.N. (1982), "Use of the balanced bipartite weighing designs." Comm. Statist. Theory Methods **11**, 769–785.

Małgorzata Graczyk

OPTYMALNE CHEMICZNE UKŁADY WAGOWE DLA $p = v + 1$ OBIEKTÓW W OPARCIU O UKŁADY BLOKÓW

W pracy omówiona jest tematyka estymacji nieznanych miar p obiektów w n pomiarach w modelu chemicznego układu wagowego. Zakłada się, że każdym pomiarze nie wszystkie obiekty biorą udział. Podane zostały warunki, przy spełnieniu których istnienie chemicznego układu wagowego dla $p = v$ obiektów implikuje istnienie chemicznego układu wagowego dla $p = v + 1$ obiektów. Do konstrukcji macierzy układu optymalnego wykorzystano macierze incydencji układów zrównoważonych o blokach niekompletnych i dwudzielnych układów bloków.