Kybernetika

Bronisław Ceranka; Małgorzata Graczyk

Optimal chemical balance weighing designs for $v + 1$ objects

Terms of use:

OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS FOR $v + 1$ OBJECTS[1]

Bronisław Ceranka and Małgorzata Graczyk

The paper studies the estimation problem of individual weights of objects using a chemical balance weighing design under the restriction on the number times in which each object is weighed. Conditions under which the existence of an optimum chemical balance weighing design for $p = v$ objects implies the existence of an optimum chemical balance weighing design for $p = v + 1$ objects are given. The existence of an optimum chemical balance weighing design for $p = v + 1$ objects implies the existence of an optimum chemical balance weighing design for each $p < v + 1$. The new construction method for optimum chemical balance weighing design for $p = v + 1$ objects is given. It uses the incidence matrices of ternary balanced block designs for v treatments.

Keywords: chemical balance weighing design, ternary balanced block design
AMS Subject Classification: 62K15

1. INTRODUCTION

Let us consider the problem of determining the weights of p objects in n measurement operations (weighings). The manner of allocation of objects on the pans is described through columns of the $n \times p$ matrix $\mathbf{X}$. Its elements are equal to $-1, 1$ or 0 if the object is kept on the left pan, right pan or is not included in the particular measurement operation, respectively. For estimation of the unknown weights of objects we use the least squares method and we get

$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}, \tag{1.1}$$

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

$$\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1} \tag{1.2}$$

provided $\mathbf{X}'\mathbf{X}$ is nonsingular, where $\mathbf{w}$ and $\mathbf{y}$ are column vectors of the unknown weights of p objects and of the recorded results in n weighings, respectively.

---

[1] Presented at the Workshop "Perspectives in Modern Statistical Inference II" held in Brno on August 14–17, 2002.

Various aspects of chemical balance weighing designs (CBWD) have been studied by Raghavarao [9], Banerjee [1] and Shah and Sinha [11]. Hotelling [8] has shown that the minimum attainable variance for each of the estimated weights for a CBWD is σ^2/n and proved the theorem that each of the variance of the estimated weights attains the lower bound if and only if $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$. This design is called the optimum chemical balance weighing design (OCBWD). In other words, the matrix $\mathbf{X}$ of the OCBWD has as elements -1 and 1, only. In this case several methods of construction OCBWD are available in the literature. Saha and Kageyama [10] have constructed OCBWD for $p = v+1$ objects in $n = 4(r-\lambda)$ weighings from the incidence matrices of the balanced incomplete block designs for v treatments. In the same case, Ceranka and Katulska [5] have studied another method of construction.

Swamy [12], Ceranka, Katulska and Mizera [7] and Ceranka and Katulska [6] have given some results of construction CBWD under the restriction on the number of objects placed on the either pan.

In the present paper we study another method of construction of an OCBWD in the case when the design matrix $\mathbf{X}$ has elements $-1, 0$ or 1. This method uses the incidence matrices of the ternary balanced block design (TBBD) for v treatments to form the design matrix of OCBWD for $p = v+1$ objects.

2. VARIANCE LIMIT OF ESTIMATED WEIGHTS

Ceranka and Graczyk [4] showed that the minimum attainable variance for each of the estimated weights for a CBWD is σ^2/m, i.e. $\mathrm{Var}(\hat{w}_j) \geq \sigma^2/m$, $j = 1, 2, \ldots, p$, where $m = \max\{m_1, m_2, \ldots, m_p\}$, m_j is the number of times in which the jth object is weighed (number of elements equal to -1 and 1 in jth column of matrix $\mathbf{X}$).

Definition 2.1. A nonsingular CBWD is called optimal for the estimated individual weights if $\mathrm{Var}(\hat{w}_j) = \sigma^2/m$, $j = 1, 2, \ldots, p$.

Ceranka and Graczyk [4] proved the following theorem.

Theorem 2.1. A nonsingular CBWD is optimal if and only if

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

In particular case, when $m = n$ the theorem was given in Hotelling [8].

3. OPTIMUM CHEMICAL BALANCE WEIGHING DESIGNS FOR $p+1$ OBJECTS

Let $\mathbf{X}_i$ be the $n_i \times p$ matrix of CBWD for $p = v$ objects, $i = 1, 2$. Based on that matrices we want to construct the design matrix $\mathbf{X}$ of CBWD for $p = v+1$ objects. Let assume that this matrix is given in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{1}_{n_1} \\ \mathbf{X}_2 & \mathbf{0}_{n_2} \end{bmatrix}, \tag{3.1}$$

where $\mathbf{1}_{n_1}$ is the $n_1 \times 1$ column vector of the units and $\mathbf{0}_{n_2}$ is the $n_2 \times 1$ column vector of zeros. In this design we have $p = v + 1$ objects and $n = n_1 + n_2$ weighing operations.

Theorem 3.1. If $\mathbf{X}_i$ is the matrix of the $n_i \times p$ OCBWD for $p = v$ objects, $i = 1, 2$, then the $n \times p$ matrix $\mathbf{X}$ given in the form (3.1) is the matrix of the OCBWD for $p = v + 1$ objects and $n = n_1 + n_2$ measurement operations if and only if

$$\mathbf{X'}_1 \mathbf{1}_{n_1} = \mathbf{0}_p. \tag{3.2}$$

Proof. The proof is straightforward when using Theorem 2.1.   □

Let notice that the existence of the OCBWD for $p = v + 1$ objects implies the existence of the OCBWD for each $p < v + 1$ objects.

In the present paper we study some methods of construction the design matrix $\mathbf{X}$ of the OCBWD for $p = v + 1$ objects using the matrices $\mathbf{X}_1$ and $\mathbf{X}_2$ of the OCBWD for $p = v$ objects. It is based on the incidence matrices of the TBBD for $p = v$ treatments.

4. TERNARY BALANCED BLOCK DESIGNS

Let TBBD be a design consisting of b blocks, each of size k, chosen from a set of size v in such a way that each of v elements occurs r times altogether and 0, 1 or 2 times in each block and each of the distinct pairs of elements occurs λ times. Any TBBD is regular, that is, each element occurs singly in ρ_1 blocks and is repeated ρ_2 blocks, where ρ_1 and ρ_2 are constant for the design. Accordingly we write the parameters of the TBBD in the form $v, b, r, k, \lambda, \rho_1, \rho_2$. Let $\mathbf{N}$ be the incidence matrix of the TBBD. It is easy to verify that

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

5. CONSTRUCTION OF THE DESIGN MATRIX

Let $\mathbf{N}_i$ be the incidence matrix of the TBBD with the parameters v, b_i, r_i, k_i, λ_i, ρ_{1i}, ρ_{2i}, $i = 1, 2$. Now we define the matrix $\mathbf{X}$ of the CBWD as

$$\mathbf{X} = \begin{bmatrix} \mathbf{N}'_1 - \mathbf{1}_{b_1}\mathbf{1}'_v & \mathbf{1}_{b_1} \\ \mathbf{N}'_2 - \mathbf{1}_{b_2}\mathbf{1}'_v & \mathbf{0}_{b_2} \end{bmatrix}. \tag{5.1}$$

In this design we have $p = v + 1$ and $n_1 = b_1, n_2 = b_2$. Thus, each of v first column of $\mathbf{X}$ will contain $\rho_{21} + \rho_{22}$ elements equal to 1, $b_1 + b_2 - \rho_{11} - \rho_{12} - \rho_{21} - \rho_{22}$

elements equal to -1 and $\rho_{11} + \rho_{12}$ elements equal to 0. The last column of $\mathbf{X}$ will contain b_1 elements equal to 1 and b_2 elements equal to 0. Clearly, such a design implies that the ith object is weighed $b_1 + b_2 - \rho_{11} - \rho_{12}$ times, $i = 1, 2, \ldots, v$, and the $(v+1)$th object is weighed b_1 times in the $n = b_1 + b_2$ weighing operations.

From Theorems 2.1 and 3.1 we have

Theorem 5.1. A nonsingular CBWD with the matrix $\mathbf{X}$ given in the form (5.1) is optimal if and only if

$$b_1 = r_1, \tag{5.2}$$

$$b_2 = \rho_{11} + \rho_{12} \tag{5.3}$$

and

$$\lambda_1 - b_1 + b_2 - 2r_2 + \lambda_2 = 0. \tag{5.4}$$

P r o o f. The proof is straightforward when using Theorems 2.1 and 3.1. $\qquad\square$

If the CBWD given by the matrix $\mathbf{X}$ in the form (5.1) is optimal then

$$Var(\hat{w}_j) = \frac{\sigma^2}{b_1}, \quad j = 1, 2, \ldots, v + 1.$$

Now we consider the matrices $\mathbf{X}_1$ and $\mathbf{X}_2$ of OCBWD for $p = v$ objects

$$\mathbf{X}_1 = \left[\begin{array}{c} \mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' \\ \mathbf{1}_{b_1}\mathbf{1}_v' - \mathbf{N}_1' \end{array} \right]$$

and

$$\mathbf{X}_2 = \mathbf{N}_2' - \mathbf{1}_{b_2}\mathbf{1}_v'.$$

Then the design matrix $\mathbf{X}$ of CBWD in the form

$$\mathbf{X} = \left[\begin{array}{cc} \mathbf{N}_1' - \mathbf{1}_{b_1}\mathbf{1}_v' & \mathbf{1}_{b_1} \\ \mathbf{1}_{b_1}\mathbf{1}_v' - \mathbf{N}_1' & \mathbf{1}_{b_1} \\ \mathbf{N}_2' - \mathbf{1}_{b_2}\mathbf{1}_v' & \mathbf{0}_{b_2} \end{array} \right]. \tag{5.5}$$

permits for estimation $p = v + 1$ objects using $n = 2b_1 + b_2$ weighing operations. Thus, each of v first column of $\mathbf{X}$ will contain $b_1 - \rho_{11} + \rho_{22}$ elements equal to $1, b_1 + b_2 - \rho_{11} - \rho_{12} - \rho_{22}$ elements equal to -1 and $2\rho_{11} + \rho_{12}$ elements equal to 0 and the last column of $\mathbf{X}$ will contain $2b_1$ elements equal to 1 and b_2 elements equal to 0.

It is obvious that for this design condition (3.2) holds and we have:

Theorem 5.2. A nonsingular CBWD with the matrix $\mathbf{X}$ given in the form (5.5) is optimal if and only if

$$b_2 = 2\rho_{11} + \rho_{12} \tag{5.6}$$

and

$$2(b_1 - 2r_1 + \lambda_1) + (b_2 - 2r_2 + \lambda_2) = 0. \tag{5.7}$$

P r o o f. The proof is straightforward when using Theorems 2.1 and 3.1. □ .

If the CBWD given by the matrix $\mathbf{X}$ of the form (5.5) is optimal then

$$\text{Var}(\hat{w}_j) = \frac{\sigma^2}{2b_1}, \quad j = 1, 2, \ldots, v+1.$$

Finally, one can easily show that if $\mathbf{X}$ is the matrix of the OCBWD then $\mathbf{X}^* = \mathbf{DXE}$ is also optimal for $\mathbf{D} = \text{diag}(\pm 1, \ldots, \pm 1)$ of order $n \times n$ and $\mathbf{E} = \text{diag}(\pm 1, \ldots, \pm 1)$ of order $p \times p$.

6. THE TERNARY BALANCED BLOCK DESIGNS LEADING TO OPTIMAL DESIGNS

We have seen in Theorems 5.1 and 5.2 that if parameters of two TBBD satisfy the conditions $(5.2), (5.3), (5.4)$ and $(5.6), (5.7)$ then a CBWD with the design matrices $\mathbf{X}$ given by (5.1) and (5.5) are optimal. Under these conditions we have formulated a theorem following the papers of Billington and Robinson [3] and Billington [2].

Theorem 6.1. The existence of two TBBD with the parameters

(i) $v = 5$, $b_1 = 4(s+4)$, $r_1 = 4(s+4)$, $k_1 = 5$, $\lambda_1 = 2(2s+7)$, $\rho_{11} = 4(s+2)$, $\rho_{21} = 4$ and $v = 5, b_2 = 5(s+4)$, $r_2 = 3(s+4)$, $k_2 = 3$, $\lambda_2 = s+6, \rho_{12} = s+12$, $\rho_{22} = s$, $s = 1, 2, \ldots$,

(ii) $v = 5$, $b_1 = 4(s+2)$, $r_1 = 4(s+2)$, $k_1 = 5$, $\lambda_1 = 4s+7$, $\rho_{11} = 4(s+1), \rho_{21} = 2$ and $v = 5$, $b_2 = 5(s+2)$, $r_2 = 3(s+2)$, $k_2 = 3$, $\lambda_2 = s+3, \rho_{12} = s+6$, $\rho_{22} = s$, $s = 1, 2, \ldots$,

(iii) $v = 6, b_1 = 3(s+5)$, $r_1 = 3(s+5)$, $k_1 = 6$, $\lambda_1 = 3s+13$, $\rho_{11} = 3s+5$, $\rho_{21} = 5$ and $v = 6, b_2 = 2(s+5)$, $r_2 = s+5, k_2 = 3$, $\lambda_2 = 2, \rho_{12} = 5 - s, \rho_{22} = s, s = 1, 2, 3, 4$,

(iv) $v = 7, b_1 = 27$, $r_1 = 27$, $k_1 = 7$, $\lambda_1 = 25$, $\rho_{11} = 15, \rho_{21} = 6$ and $v = 7, b_2 = 21$, $r_2 = 12, k_2 = 4$, $\lambda_2 = 5, \rho_{12} = 6, \rho_{22} = 3$,

(v) $v = 9, b_1 = 3(s+4)$, $r_1 = 3(s+4), k_1 = 9$, $\lambda_1 = 3s+11, \rho_{11} = 3s+4$, $\rho_{21} = 4$ and $v = 9, b_2 = 3(s+4)$, $r_2 = 2(s+4), k_2 = 6$, $\lambda_2 = s+5, \rho_{12} = 8, \rho_{22} = s, s = 1, 2, \ldots$,

(vi) $v = 11$, $b_1 = 16$, $r_1 = 16$, $k_1 = 11$, $\lambda_1 = 15$, $\rho_{11} = 6$, $\rho_{21} = 5$ and $v = 11$, $b_2 = 11$, $r_2 = 7$, $k_2 = 7$, $\lambda_2 = 4$, $\rho_{12} = 5$, $\rho_{22} = 1$,

(vii) $v = 15, b_1 = 5(s+4)$, $r_1 = 5(s+4)$, $k_1 = 15$, $\lambda_1 = 5s + 19, \rho_{11} = 5s + 6, \rho_{21} = 7$ and $v = 15, b_2 = 3(s+4)$, $r_2 = 2(s+4), k_2 = 10$, $\lambda_2 = s + 5$, $\rho_{12} = 6 - 2s$, $\rho_{22} = 2s + 1, s = 1, 2$

implies the existence of the OCBWD with the design matrix $\mathbf{X}$ given by (5.1).

Proof. It is easy to prove that the parameters of TBBD satisfy the conditions (5.2), (5.3) and (5.4).   □

Theorem 6.2.   The existence of two TBBD with the parameters

(i) $v = 5$, $b_1 = 5(s + 1)$, $r_1 = 4(s + 1)$, $k_1 = 4$, $\lambda_1 = 3s + 2$, $\rho_{11} = 4s$, $\rho_{21} = 2$ and $v = 5, b_2 = 10(s + 1)$, $r_2 = 6(s + 1)$, $k_2 = 3$, $\lambda_2 = 2(s + 2)$, $\rho_{12} = 2(s + 5)$, $\rho_{22} = 2(s - 1)$, $s = 2, 3, \ldots,$

(ii) $v = 5$, $b_1 = 2(s+4)$, $r_1 = 2(s+4)$, $k_1 = 5$, $\lambda_1 = 2s + 7$, $\rho_{11} = 2(s+2), \rho_{21} = 2$ and $v = 5$, $b_2 = 5(s+4)$, $r_2 = 3(s+4)$, $k_2 = 3$, $\lambda_2 = s+6, \rho_{12} = s+12, \rho_{22} = s$, $s = 1, 2, \ldots,$

(iii) $v = 9$, $b_1 = 3(s + 4)$, $r_1 = 2(s + 4), k_1 = 6$, $\lambda_1 = s + 5$, $\rho_{11} = 8, \rho_{21} = s$, $s = 1, 2, \ldots$ and $v = 9$, $b_2 = u + 17$, $r_2 = u + 17$, $k_2 = 9$, $\lambda_2 = u + 15, \rho_{12} = u + 1$, $\rho_{22} = 8$, $u = 1, 2, \ldots$

implies the existence of the OCBWD with the design matrix $\mathbf{X}$ given by (5.5).

Proof. It is easy to prove that the parameters of TBBD satisfy the conditions (5.6) and (5.7).   □

7. THE EXAMPLE

Let use consider the experiment in that we determine unknown measurement of $p = 6$ objects using $n = 27$ weighing operations under the assumption that each object is weighed at least $m = 12$ times. To construct the design matrix $\mathbf{X}$ of the OCBWD we use two incidence matrices of TBBD with parameters $v = 5$, $b_1 = 12$, $r_1 = 12$, $k_1 = 5$, $\lambda_1 = 11$, $\rho_{11} = 8$, $\rho_{21} = 2$

$$
\mathbf{N}_1 = \begin{bmatrix}
1 & 2 & 0 & 0 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & 1 & 2 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 2 & 1 & 2 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 2 & 1 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & 0 & 0 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}
$$

$v = 5,\ b_2 = 15,\ r_2 = 9,\ k_2 = 3,\ \lambda_2 = 4, \rho_{12} = 7,\ \rho_{22} = 1$

$$
N_2 = \begin{bmatrix}
1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 2 & 0 & 0 & 0 & 1 \\
1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 2 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 2 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 2 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 2
\end{bmatrix}.
$$

Then we built the design matrix X of the OCBWD in the form (5.1) and we have

$$
X = \begin{bmatrix} X_{(1)} \\ X_{(2)} \end{bmatrix} \qquad \text{and}
$$

$$
X'_{(1)} = \begin{bmatrix}
0 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 1 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & -1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}
$$

$$
X'_{(2)} = \begin{bmatrix}
0 & 0 & -1 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & -1 & -1 & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & -1 & 0 & 1 & -1 & -1 & -1 \\
-1 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & 1 & -1 & -1 \\
0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 1 & -1 \\
-1 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
$$

(Received September 30, 2002.)

REFERENCES

[1] K. S. Banerjee: Weighing Designs for Chemistry, Medicine, Economics, Operations Research, Statistics. Marcel Dekker, New York 1975.

[2] E. J. Billington: Balanced n-array designs: a combinatorial survey and some new results. Ars Combin. *17A* (1984), 37–72.

[3] E. J. Billington and P. J. Robinson: A list of balanced ternary block designs with $r \leq 15$ and some necessary existence conditions. Ars Combin. *16* (1983), 235–258.

[4] B. Ceranka and M. Graczyk: Optimum chemical balance weighing designs under the restriction on weighings. Discuss. Math. *21* (2001), 111–120.

[5] B. Ceranka and K. Katulska: On some optimum chemical balance weighing designs for $v + 1$ objects. J. Japan Statist. Soc. *18* (1988), 47–50.

[6] B. Ceranka and K. Katulska: Chemical balance weighing designs under the restriction on the number of objects placed on the pans. Tatra Mt. Math. Publ. *17* (1999), 141–148.

[7] B. Ceranka, K. Katulska, and D. Mizera: The application of ternary balanced block designs to chemical balance weighing designs. Discuss. Math. *18* (1998), 179–185.

[8] H. Hotelling: Some improvements in weighing and other experimental techniques. Ann. Math. Statist. *15* (1944), 297–305.

[9] D. Raghavarao: Constructions and Combinatorial Problems in Designs of Experiments. Wiley, New York 1971.

[10] G. M. Saha and S. Kageyama: Balanced arrays and weighing designs. Austral. J. Statist. *26* (1984), 119–124.

[11] K. R. Shah and B. L. Sinha: Theory of Optimal Designs. Springer, Berlin 1989.

[12] M. N. Swamy: Use of balanced bipartite weighing designs as chemical balance designs. Comm. Statist. Theory Methods *11* (1982), 769–785.

Dr. Bronisław Ceranka and Dr. Małgorzata Graczyk, Department of Mathematical and Statistical Methods, Agricultural University of Poznań, Wojska Polskiego 28, 60-637 Poznań. Poland.

e-mails: bronicer@owl.au.poznan.pl, magra@owl.au.poznan.pl