ACTA UNIVERSITATIS LODZIENSIS
FOLIA OECONOMICA 216, 2008

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NOTE ON THE OPTIMUM CHEMICAL BALANCE WEIGHING DESIGN FOR ODD NUMBER OF OBJECTS

ABSTRACT. The problem of the estimation of unknown weights of p objects is considered. The experiment is carry out according to the model of the chemical balance weighing design under the assumption that the measurement errors are correlated. The existence conditions determining the optimum design are presented.

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

I. INTRODUCTION

The problem comes from statistical theory of weighing designs. We consider the linear model:

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

which describe how to find unknown measurements of p objects using n weighing operations according to the design matrix $\mathbf{X}$. In the above model $\mathbf{y}$ is $n \times 1$ random column vector of the observed weights, $\mathbf{w}$ is $p \times 1$ column vector representing unknown weights of objects. $\mathbf{X}$, called a design matrix, can be interpreted as a weighing design for a two-pan scale or chemical scale. Assume p objects are to be weighed in n weighings, each one of them at most m times. Object jth is placed on the left pan of scale in the ith weighing if $x_{ij} = -1$, on the right pan if $x_{ij} = 1$ and omitted in the ith weighing if $x_{ij} = 0$, $i = 1,2,...,n,\ j = 1,2,...,p$. It is assumed that there are not systematic errors and

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they are equal negative correlated, i.e. for an $n \times 1$ random column 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 an $n \times 1$ column vector of zeros, $\mathbf{G}$ is an $n \times n$ positive definite matrix of known elements

$$\mathbf{G} = (1-\rho)\mathbf{I}_v + \rho \mathbf{1}_v \mathbf{1}_v', \qquad \frac{-1}{n-1} < \rho < 0, \tag{1}$$

$\mathrm{E}(\cdot)$ 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 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

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

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

II. THE OPTIMALITY CRITERION

The concept of optimality comes from statistical theory of weighing designs. The optimality criterions which deal to the weighing designs are considered in the literature. For details see Pukelsheim (1993), Shah and Sinha (1989), Wong and Masaro (1984). In the case $\mathbf{G} = \mathbf{I}_n$, some problems connected with the optimum chemical balance weighing designs have been studied in Hotelling (1944), Raghavarao (1971) and Banerjee (1975). In the situation when not all objects are included in each weighing operation and the errors are correlated with equal variances, the problem of existing of the optimum chemical balance weighing design was considered in Ceranka and Graczyk (2003). They gave the lower bound of variance of each of the estimators and the definition of the optimal design. Hence we have

Theorem 1 In the nonsingular chemical balance weighing design with the design matrix $\mathbf{X}$ and with the dispersion matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given in (1), we have

$$\mathrm{V}(\hat{w}_j) \geq \frac{\sigma^2(1-\rho)}{m - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}}, \qquad j = 1,2,...,p$$

where $u = \min\{u_1, u_2, ..., u_p\}$, u_j is equal to the number of elements equal to -1 in the j th column of the matrix $\mathbf{X}$.

Definition 1 Nonsingular chemical balance weighing design with the design matrix $\mathbf{X}$ and with the dispersion matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given in (1), is optimal if

$$\mathrm{V}(\hat{w}_j) = \frac{\sigma^2(1-\rho)}{m - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}}$$

for each j, $j = 1, 2, ..., p$.

Now, we can formulate the conditions determining the optimality criterion. We have

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

(i) $\mathbf{X}'\mathbf{X} = m\mathbf{I}_p - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}\left(\mathbf{I}_p - \mathbf{1}_p\mathbf{1}_p'\right)$,

(ii) $u_1 = u_2 = ... = u_p = u$

and

(iii) $\mathbf{X}'\mathbf{1}_n = \mathbf{z}_p$,

where $\mathbf{z}_p$ is the $p \times 1$ vector for which the j th element is equal to $(m-2u)$ or $-(m-2u)$.

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

III. BALANCED DESIGNS

In this section we remind the definitions of the balanced bipartite weighing design given in Huang (1976) and of the ternary balanced block design given in Billington (1984).

The balanced bipartite weighing design there is a design which describe how to replace v treatments in 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 parameters of the balanced bipartite weighing design. The parameters are not independent and they are related by the following identities

$$vr = bk,$$

$$b = \frac{\lambda_1 v(v-1)}{2k_1k_2},$$

$$\lambda_2 = \frac{\lambda_1\left[k_1(k_1-1)+k_2(k_2-1)\right]}{2k_1k_2},$$

$$r = \frac{\lambda_1 k(v-1)}{2k_1k_2}.$$

Let $\mathbf{N}^*$ be the incidence matrix of such design with elements equal to 0 or 1, then

$$\mathbf{N}^*\mathbf{N}^{*'} = (r-\lambda_1-\lambda_2)\mathbf{I}_v + (\lambda_1+\lambda_2)\mathbf{1}_v\mathbf{1}_v'.$$

If in the balanced bipartite weighing design $k_1 \neq k_2$ then each object exist in $r_{(1)}$ blocks in the first subblock and in $r_{(2)}$ blocks in the second subblock, $r = r_{(1)} + r_{(2)}$. Then $r_{(1)} = \lambda_1(v-1)(2k_2)^{-1}$, $r_{(2)} = \lambda_1(v-1)(2k_1)^{-1}$.

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 appears at least ones). 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. The integers $v, b, r, k, \lambda, \rho_1, \rho_2$ are parameters of the ternary balanced block design. Let $\mathbf{N}$ be the incidence matrix of the ternary balanced block design. It is straightforward to verify that

$$vr = bk,$$

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

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

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

IV. OPTIMAL DESIGNS

Let $\mathbf{N}_1^*$ be the incidence matrix of the balanced bipartite weighing design with the parameters $v, b_1, r_1, k_{11}, k_{21}, \lambda_{11}, \lambda_{21}$. From the matrix $\mathbf{N}_1^*$ we form the matrix $\mathbf{N}_1$ by replacing k_{11} elements equal to $+1$ of each column which correspond to the elements belonging to the first subblock by -1. Thus each column of the matrix $\mathbf{N}_1$ will contain k_{11} elements equal to -1, k_{21} elements equal to $+1$ and $v - k_{11} - k_{21}$ elements equal to 0. 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

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

Lemma 1 Any chemical balance weighing design with the design matrix $\mathbf{X}$ given in (2) is nonsingular.

Proof. Since $\mathbf{G}$ is the positive definite matrix then $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}$ is nonsingular if and only if $\mathbf{X}'\mathbf{X}$ is nonsingular. Hence

$$\mathbf{X}'\mathbf{X} = (r_1 - \lambda_{21} + \lambda_{11} + r_2 + 2\rho_{22} - \lambda_2)\,\mathbf{I}_v +$$

$$+ (\lambda_{21} - \lambda_{11} + b_2 - 2r_2 + \lambda_2)\,\mathbf{1}_v\mathbf{1}_v'$$

and

$$\det(\mathbf{X}'\mathbf{X}) = (r_1 - \lambda_{21} + \lambda_{11} + r_2 + 2\rho_{22} - \lambda_2)^{v-1} \cdot$$

$$\cdot\left(\frac{r_2}{k_2}(v-k_2)^2 + \frac{(v-1)\lambda_{11}}{2k_{11}k_{21}}(k_{11}-k_{21})^2\right).$$

Because $k_{11} \neq k_{21}$ then we get the thesis.

Theorem 3 Any chemical balance weighing design with the design matrix $\mathbf{X}$ in the form (2) and with the dispersion matrix $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given in (1), is optimal if and only if

(i) $\lambda_{21} - \lambda_{11} + b_2 + \lambda_2 - 2r_2 < 0$

and

(ii) $\rho = \dfrac{\lambda_{21} - \lambda_{11} + b_2 + \lambda_2 - 2r_2}{\left(r_{(21)} - r_{(11)} + r_2 - b_2\right)^2 - (b_1 + b_2 - 1)(\lambda_{21} - \lambda_{11} + b_2 + \lambda_2 - 2r_2)}$.

Proof. It is the consequence of the Lemma 1 and the Theorem 2.

From Theorem 3.4 of Huang (1976) and Theorem 1.1 of Billington and Robinson (1983) (see also Ceranka and Graczyk (2004a, 2004b)) we have

Theorem 4 If for $\rho = -\left(4st^2 - t^2 - 5t + 4st + 4\right)^{-1}$ the parameters of the balanced bipartite weighing design are equal to $v = 2t(2s-1)+1$, $b_1 = t(2t(2s-1)+1)$, $r_1 = t(4s-1)$, $k_{11} = 2s-1$, $k_{21} = 2s$, $\lambda_{11} = 2s$, $\lambda_{21} = 2s-1$ and the parameters of the ternary balanced block design are equal to $v = b_2 = 2t(2s-1)+1$, $r_2 = k_2 = 2t(2s-1)-1$, $\lambda_2 = \rho_{12} = 2t(2s-1)-3$, $\rho_{22} = 1$, $s,t = 1,2,\ldots$, $st \geq 2$, then $\mathbf{X}$ in the form (2) 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 given in (1).

From Theorem 3.4 of Huang (1976) and Lemma 2.8 of Billington and Robinson (1983) we have

Theorem 5 If for $\rho = -2\left(8st^2 - 3t^2 - 2t + 8st\right)^{-1}$ the parameters of the balanced bipartite weighing design are equal to $v = 2t(2s-1)+1$, $b_1 = t(2t(2s-1)+1)$, $r_1 = t(4s-1)$, $k_{11} = 2s-1$, $k_{21} = \lambda_{11} = 2s$, $\lambda_{21} = 2s-1$ and the parameters of the ternary balanced block design are equal to

$v = b_2 = r_2 = k_2 = 2t(2s-1)+1$, $\lambda_2 = 2t(2s-1)$, $\rho_{12} = 1$, $\rho_{22} = t(2s-1)$, $s,t = 1,2,...,$ $st \geq 2$, then **X** in the form (2) is the design matrix of the optimum chemical balance weighing design with the dispersion matrix of errors $\sigma^2\mathbf{G}$, where **G** is given in (1).

From Theorem 3.4 of Huang (1976), Theorem 4.4.3 of Billington (1984) and Theorem 2 of Saha (1975) we have

Theorem 6 If for a given ρ the parameters of the balanced bipartite weighing design are equal to $v = 2t(2s-1)+1$, $b_1 = t(2t(2s-1)+1)$, $r_1 = t(4s-1)$, $k_{11} = 2s-1$, $k_{21} = \lambda_{11} = 2s$, $\lambda_{21} = 2s-1$ and the parameters of the ternary balanced block design are equal to

(i) $\rho = -3(12st^2 - 5t^2 - 9t + 24st + 3)^{-1}$, $v = k_2 = 2t(2s-1)+1$,
$b_2 = r_2 = 2(2t(2s-1)+1)$, $\lambda_2 = 4t(2s-1)$, $\rho_{12} = 2,$, $\rho_{22} = 2t(2s-1)$,

(ii) $\rho = -3(12st^2 - 5t^2 - 21t + 48st + 15)^{-1}$, $v = k_2 = 2t(2s-1)+1$,
$b_2 = r_2 = 2(4t(2s-1)+3)$, $\lambda_2 = 4(2t(2s-1)+1)$,
$\rho_{12} = 2(2t(2s-1)+3)$, $\rho_{22} = 2t(2s-1)$,

(iii) $\rho = -3(12st^2 - 5t^2 - 21t + 48st - 9)^{-1}$, $v = k_2 = 2t(2s-1)+1$,
$b_2 = r_2 = 2(4t(2s-1)-1)$, $\lambda_2 = 4(2t(2s-1)-1)$,
$\rho_{12} = 2(2t(2s-1)-1)$, $\rho_{22} = 2t(2s-1)$,

(iv) $\rho = -(4st^2 - t^2 + t + 16st + 19)^{-1}$, $v = 2t(2s-1)+1$,
$b_2 = 4(2t(2s-1)+1)$, $r_2 = 8(t(2s-1)+1)$, $k_2 = 2(t(2s-1)+1)$,
$\lambda_2 = 4(2t(2s-1)+3)$, $\rho_{12} = 8t(2s-1)$, $\rho_{22} = 4$,

(v) $\rho = -(4st^2 - t^2 + 9t + 16st + 67)^{-1}$, $v = 2t(2s-1)+1$,
$b_2 = 4(2t(2s-1)+1)$, $r_2 = 4(2t(2s-1)-1)$, $k_2 = 2t(2s-1)-1$,
$\lambda_2 = \rho_{12} = 4(2t(2s-1)-3)$, $\rho_{22} = 4$,

(vi) $\rho = -3(12st^2 - 5t^2 - 21t + 48st + 9)^{-1}$, $v = k_2 = 2t(2s-1)+1$,
$b_2 = r_2 = 4(2t(2s-1)+1)$, $\lambda_2 = 2(4t(2s-1)+1)$, $\rho_{12} = 4(t(2s-1)+1)$,
$\rho_{22} = 2t(2s-1)$,

(vii) $\rho=-3\left(12st^2-5t^2-21t+48st+15\right)^{-1}$, $v=k_2=2t(2s-1)+1$,

$b_2=r_2=2\left(4t(2s-1)+3\right)$, $\lambda_2=4\left(2t(2s-1)+1\right)$,

$\rho_{12}=2\left(2t(2s-1)+3\right)$, $\rho_{22}=2t(2s-1)$,

(viii) $\rho=-3\left(12st^2-5t^2-21t+48st+21\right)^{-1}$, $v=k_2=2t(2s-1)+1$,

$b_2=r_2=8\left(t(2s-1)+1\right)$, $\lambda_2=2\left(4t(2s-1)+3\right)$,

$\rho_{12}=4\left(t(2s-1)+2\right)$, $\rho_{22}=2t(2s-1)$,

(ix) $\rho=-\left(4st^2-t^2-t+8st+5\right)^{-1}$, $v=k_2=2t(2s-1)+1$,

$b_2=2\left(2t(2s-1)+1\right)$, $r_2=4\left(t(2s-1)+1\right)$, $\lambda_2=2\left(2t(2s-1)+3\right)$,

$\rho_{12}=4t(2s-1)$, $\rho_{22}=2$,

(x) $\rho=-\left(4st^2-t^2+t+16st+19\right)^{-1}$, $v=2t(2s-1)+1$,

$b_2=4\left(2t(2s-1)+1\right)$, $r_2=8\left(t(2s-1)+1\right)$, $k_2=2\left(t(2s-1)+1\right)$,

$\lambda_2=4\left(2t(2s-1)+3\right)$, $\rho_{12}=8t(2s-1)$, $\rho_{22}=4$,

where $s,t=1,2,\ldots$, $st\geq 2$, then $\mathbf{X}$ in the form (2) 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 given in (1).

From Theorem 3.4 of Huang (1976) and Theorem 2.9 of Ceranka and Graczyk (2004a) we have

Theorem 7 If for $\rho=-3\left(12st^2-5t^2-9t+24st+3u\right)^{-1}$ the parameters of the balanced bipartite weighing design are equal to $v=2t(2s-1)+1$, $b_1=t\left(2t(2s-1)+1\right)$ $r_1=t(4s-1)$, $k_{11}=2s-1$, $k_{21}=\lambda_{11}=2s$, $\lambda_{21}=2s-1$ and the parameters of the ternary balanced block design are equal to $v=k_2=2t(2s-1)+1$, $b_2=r_2=8st-4t+u+1$, $\lambda_2=8st-4t+u-1$, $\rho_{12}=2st-t+1$, $\rho_{22}=2t(2s-1)$, $s,t,u=1,2,\ldots$, $st\geq 2$, then $\mathbf{X}$ in the form (2) 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 given in (1).

From Theorem 3.4 of Huang (1976) and Theorem 2.10 of Ceranka and Graczyk (2004a) we have

Theorem 8 If for ρ the parameters of the balanced bipartite weighing design are equal to $v=2t(2s-1)+1$, $b_1=t(2t(2s-1)+1)$ $r_1=t(4s-1)$, $k_{11}=2s-1$, $k_{21}=\lambda_{11}=2s$, $\lambda_{21}=2s-1$ and the parameters of the ternary balanced block design are equal to

(i) $\rho=-\left(4u^2+4st^2-t^2+t+4stu-6tu+u-1\right)^{-1}$, $v=2t(2s-1)+1$,

$b_2=u(2t(2s-1)+1)$, $r_2=u(2t(2s-1)-1)$, $k_2=2t(2s-1)-1$,

$\lambda_2=\rho_{12}=u(2t(2s-1)-3)$, $\rho_{22}=u$, $s,t,u=1,2,...,$ $st\geq 2$,

(ii) $\rho=-\left(9u^2+4st^2-t^2+t+4stu-8tu+u-1\right)^{-1}$, $v=2t(2s-1)+1$,

$b_2=u(2t(2s-1)+1)$, $r_2=2u(t(2s-1)-1)$, $k_2=2(t(2s-1)-1)$,

$\lambda_2=u(2t(2s-1)-5)$, $\rho_{12}=u(2t(2s-1)-8)$, $\rho_{22}=2u(t(2s-1)-4)$,

$s,t=2,3,...,$ $st\geq 6$, $u=1,2,...,$

(iii) $\rho=-\left(16u^2+4st^2-t^2+t+4stu-10tu+u-1\right)^{-1}$, $v=2t(2s-1)+1$,

$b_2=u(2t(2s-1)+1)$, $r_2=u(2t(2s-1)-3)$, $k_2=2t(2s-1)-3$,

$\lambda_2=u(2t(2s-1)-7)$, $\rho_{12}=u(2t(2s-1)-15)$, $\rho_{22}=6u$,

$s,t=2,3,...,$ $st\geq 6$, $u=1,2,...,$

then $\mathbf{X}$ in the form (2) 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 given in (1).

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UWAGI O OPTYMALNYCH CHEMICZNYCH UKŁADACH WAGOWYCH DLA NIEPARZYSTEJ LICZBY OBIEKTÓW

W pracy omawiany jest problem estymacji nieznanych miar obiektów w modelu chemicznego układu wagowego przy założeniu, że błędy pomiarów są skorelowane. Zostały podane warunki określające istnienie powyższych układów. Do konstrukcji macierzy układu wykorzystuje się macierze incydencji dwudzielnych układów bloków i trójkowych zrównoważonych układów bloków.