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A-Optimal Chemical Balance Weighing Design under Certain Condition

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Abstract

The paper is studying the estimation problem of individual weights of p objects using the design matrix $\mathbf{X}$ of the A-optimal chemical balance weighing design under the restriction $p_1 + p_2 = q \leq p$, where p_1 and p_2 represent the number of objects placed on the left pan and on the right pan, respectively, in each of the measurement operations. The lower bound of $\mathrm{tr}(\mathbf{X}^{'}\mathbf{X})^{-1}$ is attained and the necessary and sufficient conditions for this lower bound to be obtained are given. There are given new construction methods of the A-optimal chemical balance weighing designs based on incidence matrices of the balanced bipartite weighing designs and the ternary balanced block designs.

1 Introduction

Suppose specifically that there are p objects of true unknown weights $w_1, w_2, ..., w_p$, respectively, and we wish to estimate them employing n measuring operations using a chemical balance. Let $y_1, y_2, ..., y_n$ denote the recorded observations in these n operations, respectively. It is assumed that the observations follow the standard linear model

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e},\ \mathrm{E}(\mathbf{e}) = \mathbf{0}_n,\ \mathrm{E}(\mathbf{e}\mathbf{e}^{'}) = \sigma^2\mathbf{I}_n, \tag{1.1}$$

where $\mathbf{X}$ is of order $n \times p$ and is called the weighing design matrix. The elements of $\mathbf{X}$ are $x_{ij},\ i = 1, 2, .., n,\ j = 1, 2, ..., p,$ and a typical element x_{ij} is -1 if the jth object is placed on the left pan during the ith weighing operation, $+1$ if the jth object is placed on the right pan during the ith weighing operation and 0 if the jth object is not utilized in either pan during the ith weighing operation. Hence $\mathbf{w} = (w_1, w_2, .., w_p)^{'}$ is the vector of true unknown weights (of parameters). The vector $\mathbf{e}$ is the so-called vector of error components satisfying the usual homoscedasticy conditions.
The inference problem centres around estimation of true individual weights of all objects. The optimality problem is concerned with efficient estimation in some sense by a proper choice of the design matrix $\mathbf{X}$ among designs at our disposal. The model (1.1) is the

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standard Gauss - Markov model and the following results are well known. The parameter vector $\mathbf{w}$ is estimable if and only if $\mathrm{r}(\mathbf{X}) = p$ in which case

$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}, \quad \mathbf{V}(\hat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}, \tag{1.2}$$

where $\hat{\mathbf{w}}$ is the blue and $\mathbf{V}$ is the dispersion matrix.
In the literature some optimality criterions, i.e. A-, D-, E-optimality, are considered. Some construction methods of optimal designs are known. They are formulated for design matrices with elements equal to -1 and 1, only and they are based on incidence matrices of block designs.
Some problems connected with the optimality of chemical balance weighing designs were considered in the books of Raghavarao (1971), Banerjee (1975), Shah and Sinha (1989). Among all possible designs an A-optimal design are considered. There are designs in which the sum of variances of esimators, or equivalently $\mathrm{tr}\,(\mathbf{V}(\hat{\mathbf{w}})) = \sigma^2\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1}$, is minimal. Wong and Masaro (1984) gave the lower bound for $\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1}$ and some construction methods of the A-optimal chemical balance weighing designs.
In the paper we consider A-optimal criterion for designs for which in each measurement operation not all objects are included. In other words, in each column of the design matrix exist elements equal to -1, 1 and 0.
In the next section we give a lower bound for $\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1}$ and the necessary and sufficient conditions to this lower bound to be attained under given restriction on the number of objects included in the particular measurement operation. We present new construction method of the A-optimal design based on balanced bipartite weighing designs and ternary balanced block designs.

2 Some results on A-optimality

Let $\mathbf{X}$ be an $n \times p$ design matrix of a chemical balance weighing design. The following results from the paper Wong and Masaro (1984) give the lower bound for $\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1}$

Lemma 1 *For an $n \times p$ design matrix $\mathbf{X}$ of rank p we have the inequality*

$$\mathrm{tr}\left[(\mathbf{X}'\mathbf{X})^{-1}\right] \geq \frac{p^2}{\mathrm{tr}(\mathbf{X}'\mathbf{X})},$$

the equality being attained if and only if $\mathbf{X}'\mathbf{X}$ is equal to the $p \times p$ identity matrix $\mathbf{I}_p$ multiplied by scalar, i.e. $\mathbf{X}'\mathbf{X} = z\mathbf{I}_p$.

The lower bound of $\mathrm{tr}\left[(\mathbf{X}'\mathbf{X})^{-1}\right]$ is attained if and only if the elements of the design matrix $\mathbf{X}$ are equal to -1 or 1, only. It implies that in each measurement operation all objects must be included in different combinations. Some times it is not possible. Therefore in the present paper we consider the situation the elements of the design matrix $\mathbf{X}$ are equal to 0, either. It other words, in each weighing not all objects are included. Thus we give new lower bound of $\mathrm{tr}\left[(\mathbf{X}'\mathbf{X})^{-1}\right]$. We have

Theorem *1 For any nonsingular chemical balance weighing design with the design matrix* $\mathbf{X} = (x_{ij})$ *we have*

$$\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1} \geq \frac{p^2}{q \cdot n}, \tag{2.1}$$

where $q = \max(q_1, q_2, ..., q_n)$, $\quad q_i = \sum_{j=1}^{p} x_{ij}^2, \quad i = 1, 2, .., n.$

Proof. Because the design matrix $\mathbf{X}$ is of full column rank we have

$$\mathrm{tr}(\mathbf{X}'\mathbf{X}) = \sum_{i=1}^{n}\sum_{j=1}^{p} x_{ij}^2 = \sum_{i=1}^{n} q_i \leq q \cdot n. \tag{2.2}$$

Thus, from Lemma 1 we get (2.2). Hence the result.

In the case $q = p$ we get the inequality given in Wong and Masaro (1984).

Definition *1 Any nonsingular chemical balance weighing design with the design matrix* $\mathbf{X} = (x_{ij})$ *is said to be A-optimal if*

$$\mathrm{tr}(\mathbf{X}'\mathbf{X})^{-1} = \frac{p^2}{q \cdot n}.$$

Theorem *2 Any nonsingular chemical balance weighing design with the design matrix* $\mathbf{X} = (x_{ij})$ *is A-optimal if and only if*

$$\mathbf{X}'\mathbf{X} = \frac{q \cdot n}{p}\mathbf{I}_p.$$

Proof. To prove the necessity part we observe that from Lemma 1 we have $\mathbf{X}'\mathbf{X} = z\mathbf{I}_p$ and the equality in (2.1) is satisfied if and only if $\mathrm{tr}(\mathbf{X}'\mathbf{X}) = q \cdot n$. It implies that $z = \frac{q \cdot n}{p}$. The sufficiency part is obvious.

In the present paper we will construct an A-optimal chemical balance weighing design under the restriction $p_1 + p_2 = q \leq p$, where p_1 and p_2 represent the number of objects placed on the left and on the right pan, respectively, in each of the measurement operations. They are based on the incidence matrices of the balanced bipartite weighing designs and the ternary balanced block designs.

3 Balanced designs

In this section we recall the definitions of the balanced bipartite weighing design given in Huang (1976) and of the ternary balanced block design given in Billington (1984).
A balanced bipartite weighing design is a design which describes 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 the 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 $v,\ b,\ r,\ k_1,\ k_2,\ \lambda_1,\ \lambda_2$ are all parameters of the balanced bipartite weighing design. The parameters are not independent. They are related by the following identities

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

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

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

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 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 **N** be the incidence matrix of the ternary balanced block design. It is straightforward to verify that

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

4 Construction of the design matrix

Let $\mathbf{N}^*$ be the incidence matrix of the balanced bipartite weighing design with the parameters $v,\ b,\ r,\ k_1,\ k_2,\ \lambda_1,\ \lambda_2$. From the matrix $\mathbf{N}^*$ we form the matrix $\mathbf{N}$ by replacing k_1 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 $\mathbf{N}$ will contain k_1 elements equal to -1 and k_2 elements equal to $+1$. From the matrix $\mathbf{N}$ we construct the design matrix $\mathbf{X}$ of the chemical balance weighing design in the form $\mathbf{X} = \mathbf{N}^{'}$. In this design $p = v$ and $n = b$. The following result is from Ceranka and Graczyk (2002)

Lemma 2 *Any chemical balance weighing design with the design matrix* $\mathbf{X} = \mathbf{N}^{'}$ *is nonsingular if and only if* $k_1 \neq k_2$.

Theorem 3 *Any nonsingular chemical balance weighing design with the design matrix* $\mathbf{X} = \mathbf{N}^{'}$ *is A-optimal if and only if*

$$\lambda_2 = \lambda_1 \tag{4.1}$$

and

$$q = k. \tag{4.2}$$

Proof. For the design matrix $\mathbf{X} = \mathbf{N}'$ we have

$$\mathbf{X}'\mathbf{X} = (r - \lambda_2 + \lambda_1)\mathbf{I}_v + (\lambda_2 - \lambda_1)\mathbf{1}_v\mathbf{1}_v'$$

and

$$\mathbf{X}'\mathbf{X} = \tfrac{q \cdot b}{v}\mathbf{I}_v.$$

Comparing these two equalities we get $\lambda_2 = \lambda_1$ and $r - \lambda_2 + \lambda_1 = \frac{q \cdot b}{v}$. If (4.1) is satisfied then we get (4.2) from the last equation. Hence we get the thesis of the Theorem.

Now, we consider the chemical balance weighing design with the design matrix $\mathbf{X} = \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v'$, where $\mathbf{N}$ is the incidence matrix of the ternary balanced block design with the parameters $v,\ b,\ r,\ k,\ \lambda,\ \rho_1,\ \rho_2$. In this design $p = v$ and $n = b$. From Ceranka, Katulska and Mizera (1998) we have

Lemma 3 *Any chemical balance weighing design with the design matrix* $\mathbf{X} = \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v'$ *is nonsingular if and only if* $v \neq k$.

Thus we get

Theorem 4 *Any nonsingular chemical balance weighing design with the design matrix* $\mathbf{X} = \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v'$ *is A-optimal if and only if*

$$b + \lambda - 2r = 0 \tag{4.3}$$

and

$$b - \rho_1 = \frac{q \cdot b}{v}. \tag{4.4}$$

Proof. For the design matrix $\mathbf{X} = \mathbf{N}' - \mathbf{1}_b\mathbf{1}_v'$ we have

$$\mathbf{X}'\mathbf{X} = (r + 2\rho_2 - \lambda)\mathbf{I}_v + (b + \lambda - 2r)\mathbf{1}_v\mathbf{1}_v'$$

and

$$\mathbf{X}'\mathbf{X} = \tfrac{q \cdot b}{v}\mathbf{I}_v.$$

Comparing these two equalities we get $b + \lambda - 2r = 0$ and $r + 2\rho_2 - \lambda = \frac{q \cdot b}{v}$. If (4.3) is satisfied we get (4.4) from the last equation. Hence the claim of the Theorem.

5 Balanced bipartite weighing designs leading to the A-optimal designs

We have seen in the Theorem 3 that if the parameters of the balanced bipartite weighing design satisfy the condition (4.1) then the chemical balance weighing design with the design matrix $\mathbf{X} = \mathbf{N}'$ is A-optimal. Under this condition we have the following Theorem given in Ceranka and Graczyk (2005)

Theorem 5 *The existence of the balanced bipartite weighing design with the parameters* $v,\ b=\frac{2sv(v-1)}{c^2(c^2-1)},\ r=\frac{2s(v-1)}{c^2-1},\ k_1=\frac{c(c-1)}{2},\ k_2=\frac{c(c+1)}{2},\ \lambda_1=s,\ \lambda_2=s,\ c=2,3,...,\ s=1,2,...$ *implies the existence of the A-optimal chemical balance weighing design,* $v\geq c^2,\ q=c^2$.

6 Ternary balanced block designs leading to the A-optimal designs

We have seen in the Theorem 4 that if the parameters of the ternary balanced block design satisfy the condition (4.3) then a chemical balance weighing design with the design matrix $\mathbf{X}=\mathbf{N}'-\mathbf{1}_b\mathbf{1}_v'$ is A-optimal. Under this condition we have the following Theorem

Theorem 6 *The existence of the ternary balanced block design with the parameters*

(i) $v=s,\ b=us,\ r=u(s-2),\ k=s-2,\ \lambda=u(s-4),\ \rho_1=u(s-4),\ \rho_2=u,\ u=1,2,...,\ s=5,6,...,$ *except the case* $u=1$ *and* $s=5$,

(ii) $v=s,\ b=us,\ r=u(s-3),\ k=s-3,\ \lambda=u(s-6),\ \rho_1=u(s-9),\ \rho_2=3u,\ u=1,2,...,\ s=10,11,...,$

(iii) $v=s,\ b=us,\ r=u(s-4),\ k=s-4,\ \lambda=u(s-8),\ \rho_1=u(s-16),\ \rho_2=6u,\ u=1,2,...,\ s=17,18,...,$

implies the existence of the A-optimal chemical balance weighing design.

Proof. It is easy to see that the parameters (i)-(iii) satisfy the conditions (4.3) and (4.4).

Example We determine unknown measurements of $p=6$ objects by weighing them $n=6$ times and each object is weighed at most $q=4$ times. For construction the design we consider the ternary balanced block design with the parameters $v=b=6,\ r=k=4,\ \lambda=\rho_1=2,\ \rho_2=1$ (see Theorem 6(i)) and with the incidence matrix

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

Based on the matrix $\mathbf{N}$ we form the design matrix $\mathbf{X}$ of the A-optimal chemical balance weighing design in the form $\mathbf{X}=\mathbf{N}'-\mathbf{1}_b\mathbf{1}_v'$

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & -1 & -1 & 0 & -1 \\ -1 & 1 & 0 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 & -1 & -1 \\ -1 & 0 & -1 & 1 & 0 & -1 \\ -1 & -1 & 0 & -1 & 1 & 0 \\ 0 & -1 & -1 & 0 & -1 & 1 \end{bmatrix}.$$

We have $\mathbf{X}'\mathbf{X} = 4\mathbf{I}_6$ and $\mathrm{V}(\hat{w}_i) = \frac{\sigma^2}{4}$ for $i = 1, 2, ..., 6$.

In the paper were presented conditions determined A-optimal chemical balance weighing design and some new methods of construction of designs under assumption no all objects are included in each measurement operation. These methods are based on the incidence matrices of balanced bipartite weighing designs and ternary balanced block design.

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