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ON SOME CONSTRUCTION OF *D*-OPTIMAL CHEMICAL BALANCE WEIGHING DESIGNS

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Summary

In this paper, we discuss the problem of estimation of individual weights of three objects in the chemical balance weighing design using the criterion of *D*-optimality. We assume that the sequence ε_i of error terms is a first-order autoregressive process, called $AR(1)$ process. We present the *D*-optimal chemical balance weighing design $\hat{\mathbf{X}}$ in the class of designs with the design matrix $\mathbf{X} \in M_{n\times 3}(\pm 1)$ such that each column of the matrix $\mathbf{X}$ contains at least one 1 and one –1.

Key words and phrases: $AR(1)$ prosess, chemical balance weighing design, *D*-optimal design

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1. Introduction

The formulation to a weighing design problem calls for some objects with unknown weights and a weight measuring device is known as a balance. In a chemical balance, there are two pans (left and right). Any object can be placed on the left or right pan. Then the pointer provides a reading which represents the total weight of the objects on the pans. Chemical balance weighing designs are also the name for experiments which results can be described as the linear combination of unknown measurements of objects with factors of this combination equal to 1 or -1.

Assume that $n \equiv 0 \pmod 4$. There are 3 objects of the true unknown weights w_1, w_2, w_3, respectively, and we wish to estimate them employing n measuring operations using a chemical balance. Let $y_1, y_2, \ldots, y_n$ denote the observations in these n operations, respectively. We assume that the observations follow the linear model

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\varepsilon},$$

where $\mathbf{y} = [y_1, y_2, \ldots, y_n]^T$ is an $n \times 1$ vector of observations, $\mathbf{w} = [w_1, w_2, w_3]^T$ is the vector of true unknown weights (parameters) of objects, the matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & x_{n3} \end{bmatrix}$$

is called the design matrix and $x_{ij} = -1$ if the *j*th object is placed on the left pan during the *i*th weighing operation, $x_{ij} = 1$ if the *j*th object is placed on the right pan during the *i*th weighing operation, the vector $\boldsymbol{\varepsilon} = [\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n]^T$ is the so-called vector of error components such that $E(\boldsymbol{\varepsilon}) = [0, 0, \ldots, 0]^T$ is an $n \times 1$ vector of zeros and $Var(\boldsymbol{\varepsilon}) = \frac{1}{1-\rho^2}\mathbf{S}$, where

$$\mathbf{S} = \begin{bmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-2} & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-3} & \rho^{n-2} \\ \rho^2 & \rho & 1 & \cdots & \rho^{n-4} & \rho^{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho^{n-2} & \rho^{n-3} & \rho^{n-4} & \cdots & 1 & \rho \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & \rho & 1 \end{bmatrix}$$

and $-1 < \rho < 1$.

To estimate individual unknown weights of objects we use the normal equations

$$\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X}\hat{\mathbf{w}} = \mathbf{X}^T\mathbf{S}^{-1}\mathbf{y}.$$

We say that chemical balance weighing design is singular or nonsingular if the matrix $\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X}$ is singular or nonsingular, respectively. This matrix is called the information matrix for the design. If the matrix $\mathbf{X}$ is of full column rank (the design is nonsingular), then the generalized least-squares estimator of the vector $\mathbf{w}$ is given in the form

$$\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{S}^{-1}\mathbf{y}.$$

The covariance matrix of $\hat{\mathbf{w}}$ is given by the formula

$$Var(\hat{\mathbf{w}}) = \frac{1}{1-\rho^2}(\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X})^{-1}.$$

The inverse of the matrix $\mathbf{S}$ is equal to the matrix $\frac{1}{1-\rho^2}\mathbf{A}$ for $\rho \in (-1,1)$, where

$$\mathbf{A} = \begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 & 0 \\ 0 & -\rho & 1+\rho^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1+\rho^2 & -\rho \\ 0 & 0 & 0 & \cdots & -\rho & 1 \end{bmatrix}.$$

It is well known from literature (for example Horn and Johnson (1985)) that above matrix is positive definite for $\rho \in (-1,1)$.

We consider the chemical balance weighing designs which minimize the determinant of $(\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X})^{-1}$, the inverse of the information matrix $\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X}$. This condition is equivalent to maximizing the determinant of the information matrix.

Definition 1.1. We say that the design matrix $\hat{\mathbf{X}}$ is *D*-optimal in the class C of the designs matrices, where C is a subset of $M_{n\times 3}(\pm 1)$, if

$$\det(\hat{\mathbf{X}}^T\mathbf{S}^{-1}\hat{\mathbf{X}}) = \max\{\det(\mathbf{X}^T\mathbf{S}^{-1}\mathbf{X}) : \mathbf{X}\in C\},$$

where $M_{n\times m}(\pm 1)$ is the set of all matrices with n rows, m columns and each element is 1 or -1.

Hotelling (1944) studied some problems connected with chemical balance weighing designs, when the matrix $\mathbf{S}$ was the identity matrix $(\rho = 0)$. He proved that the design is optimal if its design matrix $\mathbf{X}$ is such that $\mathbf{X}^T\mathbf{X} = n\mathbf{I}_3$. For $-1<\rho<0$, Li and Yang (2005) have proved that the design with the design matrix

$$\mathbf{X}^* = \begin{bmatrix} 1 & 1 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 1 \\ 1 & 1 & -1_2 \\ \vdots & \vdots & \vdots \\ 1 & 1 & -1 \\ 1 & -1_1 & -1 \\ \vdots & \vdots & \vdots \\ 1 & -1 & -1 \\ 1 & -1 & 1_3 \\ \vdots & \vdots & \vdots \\ 1 & -1 & 1 \end{bmatrix},$$

where elements with indices $1, 2$ and 3 are in positions $\left(\frac{n}{2}+1, 2\right), \left(\frac{n}{4}+1, 3\right), \left(\frac{3n}{4}+1, 3\right)$, respectively, is *D*-optimal in the class of designs with the design matrix $\mathbf{X} = [\mathbf{1}\,|\,\mathbf{x}\,|\,\mathbf{u}] \in M_{n\times 3}(\pm 1)$, where $\mathbf{1} = [1, 1, \ldots, 1]^T$, $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$ and $\mathbf{u} = [u_1, u_2, \ldots, u_n]^T$. Yeh and Lo Huang (2005) have considered similar problems for the complete 2^k factorial designs and the 2^{k-p}

fractional factorial designs also for $0<\rho<1$ and $n \equiv 2 \pmod 4$. The *D*-optimal designs in these two papers are the conjectures from Bora-Senta and Moyssiadis (1999).

In the next section we present that the design with the design matrix

$$\hat{\mathbf{X}} = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ \vdots & \vdots & \vdots \\ -1 & 1 & 1 \\ -1 & 1 & -1_5 \\ \vdots & \vdots & \vdots \\ -1 & 1 & -1 \\ -1 & -1_4 & -1 \\ \vdots & \vdots & \vdots \\ -1 & -1 & -1 \\ -1 & -1 & 1_6 \\ \vdots & \vdots & \vdots \\ -1 & -1 & 1 \end{bmatrix}, \tag{1.1}$$

where elements with indices 4, 5 and 6 are in positions $\left(\frac{n}{2}+2,\, 2\right), \left(\frac{n}{4}+2,\, 3\right), \left(\frac{3n}{4}+1,\, 3\right)$, respectively, is *D*-optimal in certain class of designs with the design matrix $\mathbf{X}=[\mathbf{x}\,|\,\mathbf{u}\,|\,\mathbf{v}] \in M_{n\times 3}(\pm 1)$, where $\mathbf{x}=[x_1, x_2, \ldots, x_n]^T$, $\mathbf{u}=[u_1, u_2, \ldots, u_n]^T$, $\mathbf{v}=[v_1, v_2, \ldots, v_n]^T$, such that each column of matrix $\mathbf{X}$ contains at least one 1 and one -1.

In proofs of theorems in the next section we used similar notation as in Li and Yang (2005) and Yeh and Lo Huang (2005). In particular, we used the following inequalities for the determinant formulated in Horn and Johnson (1985).

Lemma 1.1. (Hadamard's inequality). If $\mathbf{P}=[p_{ij}]$ is an $n\times n$ positive semi-definite matrix, then

$$\det(\mathbf{P}) \le \prod_{i=1}^{n} p_{ii}.$$

Futhermore, when $\mathbf{P}$ is positive definite, then equality holds if and only if $\mathbf{P}$ is diagonal.

Lemma 1.2. (Fischer's inequality). If

$$\mathbf{P} = \begin{bmatrix} \mathbf{B} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{D} \end{bmatrix}$$

is a positive definite matrix that is partitioned so that $\mathbf{B}$ and $\mathbf{D}$ are square and nonempty, then

$$\det(\mathbf{P}) \le \det(\mathbf{B})\det(\mathbf{D}).$$

2. *D*-optimal weighing designs

In this section we present new results concerning *D*-optimal chemical balance weighing designs. First we must define some notation.

For any vector $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T \in M_{n\times 1}(\pm 1)$, we define the number

$$cs(\mathbf{x}) = \#\{i : x_i = -x_{i+1}, 1 \le i \le n-1\}.$$

For example, if $\mathbf{x} = [1, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1, 1, 1, 1, 1, -1, -1, 1]^T$, then $cs(\mathbf{x}) = 4$.

For a matrix $\mathbf{X} = [\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in M_{n\times 3}(\pm 1)$ we define the function $f(\mathbf{X}) = f(\mathbf{x}, \mathbf{u}, \mathbf{v})$ by the formula

$$f(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \det(\mathbf{X}^T\mathbf{A}\mathbf{X}) = \det\begin{bmatrix} \mathbf{x}^T\mathbf{A}\mathbf{x} & \mathbf{x}^T\mathbf{A}\mathbf{u} & \mathbf{x}^T\mathbf{A}\mathbf{v} \\ \mathbf{u}^T\mathbf{A}\mathbf{x} & \mathbf{u}^T\mathbf{A}\mathbf{u} & \mathbf{u}^T\mathbf{A}\mathbf{v} \\ \mathbf{v}^T\mathbf{A}\mathbf{x} & \mathbf{v}^T\mathbf{A}\mathbf{u} & \mathbf{v}^T\mathbf{A}\mathbf{v} \end{bmatrix}.$$

The value of the above function does not change if we interchange two columns of the matrix $\mathbf{X}$ and we multiply any column of this matrix by -1. Thus the matrix which maximizes the function f is unique with the exactness to the above operations. We define also the following notation

$\Delta = \mathbf{1}^T \mathbf{A}\mathbf{1} = (1-\rho)[(n-2)(1-\rho)+2]$ and $\hat{f} = f(\hat{\mathbf{X}})$, where $\hat{\mathbf{x}}$ is given by formula (1.1).

First, we consider the special case $n = 4$. Thus $\Delta = 2(1-\rho)(2-\rho)$,

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

and

$$\hat{f} = \det \begin{bmatrix} \Delta + 4\rho & 2\rho(1-\rho) & 0 \\ 2\rho(1-\rho) & \Delta + 4\rho & -4\rho \\ 0 & -4\rho & \Delta + 8\rho \end{bmatrix} = 32(\rho^3 - \rho + 2).$$

In this case we proved the following

Theorem 2.1. Let $n = 4$ and $-1 < \rho \le 0$. If

$$[\mathbf{x} \,|\, \mathbf{u} \,|\, \mathbf{v}] \in \{[\boldsymbol{\alpha} \,|\, \boldsymbol{\beta} \,|\, \boldsymbol{\gamma}] \in M_{n\times 3}(\pm 1) : cs(\boldsymbol{\alpha}) \ge 1, cs(\boldsymbol{\beta}) \ge 1, cs(\boldsymbol{\gamma}) \ge 1\},$$

then

$$\hat{f} \ge f(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

This class of designs is very small and we are able to write out all designs. For example, when $cs(\mathbf{x}) = 1, cs(\mathbf{u}) = 1, cs(\mathbf{v}) = 2$, we consider only nine designs with design matrices given below

$$\mathbf{X}_1 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_2 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_3 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & -1 & 1 \end{bmatrix},$$

$$\mathbf{X}_4 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_5 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_6 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix},$$

$$\mathbf{X}_7 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_8 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{X}_9 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}.$$

Hence

$$f(\mathbf{X}_i) = \begin{cases} 32(\rho^2 + 1) & i = 1, 3, 7, 8 \\ 32(1-\rho) & i = 2, 4, 9 \\ 32(\rho^3 - \rho + 2) & i = 5, 6 \end{cases}.$$

Then it is easy to see that $\hat{f} \geq f(\mathbf{X}_i)$ for $i = 1, 2, \ldots, 9$.

Immediately, from the above theorem we have the following corollary.

Corollary 2.2. For $n = 4$ and $-1 < \rho \leq 0$ the design with the design matrix $\hat{\mathbf{X}}$ given by (1.1) is *D*-optimal in the class of designs with the design matrix $\mathbf{X} \in M_{4\times 3}(\pm 1)$ such that each column of the matrix $\mathbf{X}$ contains at least one 1 and one -1.

Now, suppose that $n \geq 8$ and $n \equiv 0 \pmod 4$. Therefore

$$\hat{f} = \det \begin{bmatrix} \Delta + 4\rho & 2\rho(1-\rho) & 0 \\ 2\rho(1-\rho) & \Delta + 4\rho & 0 \\ 0 & 0 & \Delta + 8\rho \end{bmatrix} =$$

$$= (\Delta + 4\rho)^2 (\Delta + 8\rho) - 4\rho^2 (1-\rho)^2 (\Delta + 8\rho).$$

In proof of the below theorem, we used the Hadamard and Fischer inequalities.

Theorem 2.3. Let $n = 4\theta, \theta = 2, 3, \ldots$ and $-1 < \rho \le 0$. If

$$[\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in \{[\boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 3}(\pm 1) : cs(\boldsymbol{\alpha}) \ge 1, cs(\boldsymbol{\beta}) \ge 1, cs(\boldsymbol{\gamma}) \ge 2\},$$

then

$$\hat{f} \ge f(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

Corollary 2.4. For $n \equiv 0 \pmod 4$ and $-1 < \rho \le 0$ the design with the design matrix $\hat{\mathbf{X}}$ given by (1.1) is *D*-optimal in the class of designs with the design matrix $\mathbf{X} = [\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in M_{n\times 3}(\pm 1)$ such that $cs(\mathbf{x}) \ge 1, cs(\mathbf{u}) \ge 1, cs(\mathbf{v}) \ge 2$.

In the case, when we consider the class of the designs with the design matrices $\mathbf{X} = [\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in M_{n\times 3}(\pm 1)$ such that $cs(\mathbf{x}) \ge 1, cs(\mathbf{u}) \ge 1, cs(\mathbf{v}) \ge 1$ we obtained (using Fischer's inequality) weaker theorem as in Yeh and Lo Huang (2005).

Theorem 2.5. Let $n = 4\theta, \theta = 2, 3, \ldots$ and $\dfrac{-1}{n+1} \le \rho \le 0$. If

$$[\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in \{[\boldsymbol{\alpha} \mid \boldsymbol{\beta} \mid \boldsymbol{\gamma}] \in M_{n\times 3}(\pm 1) : cs(\boldsymbol{\alpha}) \ge 1, cs(\boldsymbol{\beta}) \ge 1, cs(\boldsymbol{\gamma}) \ge 1\},$$

then

$$\hat{f} \ge f(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

Therefore, in the class of designs with the design matrix $\mathbf{X} \in M_{n\times 3}(\pm 1)$ such that each column of matrix $\mathbf{X}$ contains at least one 1 and one -1 we have the below corollary.

Corollary 2.6. For $n \equiv 0 \pmod 4$ and $-1/(n+1) \le \rho \le 0$ the design with the design matrix $\hat{\mathbf{X}}$ given by (1.1) is *D*-optimal in the class of designs with the design matrix $\mathbf{X} = [\mathbf{x} \mid \mathbf{u} \mid \mathbf{v}] \in M_{n\times 3}(\pm 1)$ such that $cs(\mathbf{x}) \ge 1, cs(\mathbf{u}) \ge 1, cs(\mathbf{v}) \ge 1$.

It is easy to see that when $\rho = 0$ the matrix $\mathbf{S}$ is the identity matrix. This case is well known in literature (see Hotelling, 1944 or Galil and Kiefer, 1980). Results present in this paper for $\rho = 0$ are consistent with results in literature.

3. Conclusion

We considered *D*-optimality problem if $\rho \in (-1, 0]$ and $p = 3$. We believe that the techniques presented in this paper could be extended to resolve this problem for $p > 3$. For the present this problem is open.

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O PEWNEJ KONSTRUKCJI *D*-OPTYMALNYCH CHEMICZNYCH UKŁADÓW WAGOWYCH

Streszczenie

W niniejszej pracy dyskutowany jest problem estymacji miar obiektów w chemicznym układzie wagowym w oparciu o kryterium *D*-optymalności. Zakłada się, że błędy losowe tworzą proces autoregresyjny rzędu pierwszego, zwany procesem $AR(1)$. Pokazano, że układ o macierzy układu $\hat{\mathbf{X}}$ dany wzorem (1.1) jest *D*-optymalny w pewnej klasie układów o macierzy układu $\mathbf{X} \in M_{n\times 3}(\pm 1)$ takiej, że każda kolumna macierzy $\mathbf{X}$ zawiera przynajmniej jeden element równy 1 oraz jeden równy -1.

Słowa kluczowe: chemiczne układy wagowe, *D*-optymalne układy, proces *AR*(1)

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