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A NOTE ON D−EFFICIENCY OF BIASED CHEMICAL BALANCE WEIGHING DESIGNS

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Summary

In this paper, the D-efficiency of biased chemical balance weighing designs for the estimation of individual unknown weights of objects is considered. The error components are assumed to create a first-order autoregressive process. Then the covariance matrix of error terms has known form, which does not have to be identity matrix and it depends on the known parameter ρ. When the number of observations $n \equiv 0(mod4)$ Katulska and Smaga (2011) showed that some designs are D-optimal biased designs, if the number of objects is three and $\rho \in [0,1/(n-2)]$. In this paper the lower bound for D-efficiency of biased chemical balance weighing designs with three objects is given for all $\rho \in [1/(n-2),1]$ and $n \equiv 0(mod4)$. Moreover, using that lower bound for D-efficiency, it is shown that the designs constructed in Katulska and Smaga (2011) are highly D-efficient when $\rho \in [1/(n-2),1]$ and $n \equiv 0(mod4)$.

Keywords and phrases: biased chemical balance weighing design, D-efficiency, first-order autoregressive process

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1. Introduction

Let us introduce the model of the chemical balance weighing design. There are p objects of the true unknown weights $w_1, w_2, \ldots, w_p$, respectively. Weights are estimated employing n measuring operations using a chemical balance. Suppose that $y_1, y_2, \ldots, y_n$ 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 $\mathbf{y} = [y_1, y_2, \ldots, y_n]'$ is a vector of observations, $\mathbf{w} = [w_1, w_2, \ldots, w_p]'$ is the vector of unknown weights of objects, $\mathbf{X} = [x_{ij}]$ is an $n \times p$ design matrix and $x_{ij} = -1$ $(x_{ij} = 1)$ if the jth object is placed on the left (right) pan during the ith weighing operation, $\boldsymbol{\varepsilon} = [\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n]'$ is the vector of error terms such that $\mathrm{E}(\boldsymbol{\varepsilon}) = [0, 0, \ldots, 0]'$ is the $n \times 1$ null vector and

$$\mathrm{Var}(\boldsymbol{\varepsilon}) = \frac{1}{1-\rho^2}\mathbf{S},$$

where $\mathbf{S} = (\rho^{|r-d|})_{r,d=1}^{n}$ and $-1 < \rho < 1$. The weighing design is identified with its design matrix $\mathbf{X}$. When the first column of a design matrix $\mathbf{X}$ contains only ones, such design is called a biased chemical balance weighing design with $p-1$ objects.

The vector of unknown parameters $\mathbf{w}$ is estimated using the normal equations, i.e.

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

The chemical balance weighing design is singular (nonsingular) if the information matrix $\mathbf{X}'\mathbf{S}^{-1}\mathbf{X}$ is singular (nonsingular). When the design is nonsingular, the generalized least-squares estimator of $\mathbf{w}$ is of the form

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

and its covariance matrix is equal to

$$\mathrm{Var}(\hat{\mathbf{w}}) = \frac{1}{1-\rho^2}(\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})^{-1},$$

where $\mathbf{S}^{-1} = 1/(1-\rho^2)\mathbf{A}$ and

$$\mathbf{A} = \begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 & 0 \\ 0 & -\rho & 1+\rho^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1+\rho^2 & -\rho \\ 0 & 0 & 0 & \cdots & -\rho & 1 \end{bmatrix} \tag{1.1}$$

is positive definite matrix for $\rho \in (-1, 1)$.

We would like to choose a chemical balance weighing design that is optimal or nearly optimal with respect to some criterion. In the literature, several optimality criteria of measure the quality of weighing designs are considered. We are interested in the D-optimal chemical balance weighing designs, which maximize the determinant of the information matrix, i.e., the design $\tilde{\mathbf{X}}$ is D-optimal in the class C, where C is a subset of the set $M_{n\times p}(\pm 1)$ of all matrices with n rows, p columns and elements 1 or -1, if

$$\det(\tilde{\mathbf{X}}'\mathbf{S}^{-1}\tilde{\mathbf{X}}) = \max\{\det(\mathbf{X}'\mathbf{S}^{-1}\mathbf{X}) : \mathbf{X} \in C\}.$$

Since $\mathbf{S}^{-1} = 1/(1-\rho^2)\mathbf{A}$, the design $\tilde{\mathbf{X}}$ is D-optimal in the class $C \subseteq M_{n\times p}(\pm 1)$, if

$$\det(\tilde{\mathbf{X}}'\mathbf{A}\tilde{\mathbf{X}}) = \max\{\det(\mathbf{X}'\mathbf{A}\mathbf{X}) : \mathbf{X} \in C\},$$

where $\mathbf{A}$ is of the form (1.1).

When the error terms have a normal distribution, D-optimal design minimizes the expected volume of the usual confidence ellipsoid for the vector of parameters $\mathbf{w}$.

In the case when $\rho = 0$ (the matrix $\mathbf{S}$ is the identity matrix), D-optimal designs are considered in many papers (see, for example, Cheng (2014), Galil and Kiefer (1980), or Jacroux et al. (1983)). For $\rho \neq 0$, Katulska and Smaga (2011, 2012, 2013), Li and Yang (2005), Yeh and Lo Huang (2005) and Smaga (to appear) showed some results about D-optimal designs and D-optimal biased designs, if $p = 3$ or $p = 4$. There are also considered optimal designs with some other forms of the covariance matrix of the vector of error components (see, for example, Ceranka et al. (2006), Graczyk (2012), or Masaro and Wong (2008)). Some applications of optimal weighing designs are given in Cheng (2014) and Graczyk (2013). Jenkins and Chanmugam (1962) considered an experiment connected with a chemical process planed by a chemical balance weighing design. The observations were described by a model with autocorrelation ($\rho \neq 0$). They also give an illustrative example. In Katulska and Smaga (2011), the following theorem is proved.

Theorem 1.1 (Katulska and Smaga (2011)). Let $\rho \in [0, 1/(n-2)]$ and $n \equiv 0 \pmod 4$. The design

$$\hat{\mathbf{X}} = \left[\mathbf{1}_n \,|\, \mathbf{1}_{n/2} \otimes [1, -1]' \,|\, \hat{\mathbf{x}} \,|\, \hat{\mathbf{y}}\right], \tag{1.2}$$

where $\otimes$ denotes the Kronecker product, $\hat{\mathbf{x}}' = \left[\mathbf{1}'_{n/4} \otimes [1, -1], \mathbf{1}'_{n/4} \otimes [-1, 1]\right]$ and

$$\hat{\mathbf{y}}' = \begin{cases} \left[\mathbf{1}'_{(n-4)/8} \otimes [1, -1], 1, \mathbf{1}'_{n/4} \otimes [1, -1], -1, \mathbf{1}'_{(n-4)/8} \otimes [1, -1]\right] & , if \;\; n/4 = 2k-1, \\ \left[\mathbf{1}'_{n/8} \otimes [1, -1], \mathbf{1}'_{n/4} \otimes [-1, 1], \mathbf{1}'_{n/8} \otimes [1, -1]\right] & , if \;\; n/4 = 2k, \end{cases}$$

$k = 1, 2, \ldots,$ is D-optimal in the class of biased designs $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1),\;\; rank(\mathbf{X}) = 4.$

The necessary and sufficient condition under which the design is D-optimal in the class of biased weighing designs with three objects is also given in Katulska and Smaga (2011). Simulation study suggests that the designs $\hat{\mathbf{X}}$ are D-optimal for all $\rho \in [0, 1)$, not only for $\rho \in [0, 1/(n-2)]$. Moreover, when n is large, $1/(n-2)$ is close to zero and the interval for possible values of the parameter ρ, for which D-optimality of designs $\hat{\mathbf{X}}$ is proved, is narrow. In this paper, it is shown that the designs $\hat{\mathbf{X}}$ are highly D-efficient for all $\rho \in (1/(n-2), 1)$.

The remainder of this paper is organized as follows. In Section 2, we define D-efficiency of biased chemical balance weighing designs with three objects and give the lower bound for it when $\rho \in [0, 1)$. In Section 3, we study D-efficiency of designs $\hat{\mathbf{X}}$ given by (1.2) for $\rho \in (1/(n-2), 1)$ using results of Section 2.

2. The lower bound for D-efficiency

By the definition in Bulutoglu and Ryan (2009), the D-efficiency of a design $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1),$ is given by the formula

$$D-eff\,(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})}{\max\{\det(\mathbf{Y}'\mathbf{S}^{-1}\mathbf{Y}) : \mathbf{Y} = [\mathbf{1} \,|\, \mathbf{y}_1 \,|\, \mathbf{y}_2 \,|\, \mathbf{y}_3] \in M_{n\times 4}(\pm 1)\}} \right]^{1/4}.$$

The form of the inverse of the matrix $\mathbf{S}$ implies

$$D-eff\,(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{A}\mathbf{X})}{\max\{\det(\mathbf{Y}'\mathbf{A}\mathbf{Y}) : \mathbf{Y} = [\mathbf{1} \,|\, \mathbf{y}_1 \,|\, \mathbf{y}_2 \,|\, \mathbf{y}_3] \in M_{n\times 4}(\pm 1)\}} \right]^{1/4}. \quad (2.1)$$

Theorem 1.1 shows that $D-eff\,(\hat{\mathbf{X}}) = 1$ for all $\rho \in [0, 1/(n-2)]$. Unfortunately, the denominator of $D-eff\,(\mathbf{X})$ is unknown for $\rho > 1/(n-2)$. However, we give the upper bound for it in the following lemma. In the proof of this lemma, we use Fischer's inequality, which is recalled below.

Theorem 2.1 (Fischer's inequality). If

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

is a positive definite matrix that is partitioned so that $\mathbf{B}$ and $\mathbf{D}$ are square and nonempty, then $\det(\mathbf{P}) \le \det(\mathbf{B})\det(\mathbf{D})$ and the equality holds if and only if $\mathbf{C} = \mathbf{0}$.

Lemma 2.1. If $n \equiv 0 \pmod 4$, $\rho \in [0, 1)$, and $\mathbf{X} = [\mathbf{1} \,|\, \mathbf{x} \,|\, \mathbf{y} \,|\, \mathbf{z}] \in M_{n\times 4}(\pm 1)$, then

$$\det(\mathbf{X}'\mathbf{A}\mathbf{X}) \le \delta\Delta(\Delta - 4\rho)^2, \quad (2.2)$$

where $\delta = \mathbf{1}'\mathbf{A}\mathbf{1} = (n-2)(1-\rho)^2 + 2(1-\rho)$ and $\Delta = (n-2)(1+\rho)^2 + 2(1+\rho)$.

Proof. Let $\mathbf{X}=[\mathbf{1}\,|\,\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]\in M_{n\times 4}(\pm 1)$ be arbitrary. Fischer's inequality implies

$$\det(\mathbf{X}'\mathbf{A}\mathbf{X})\le(\mathbf{1}'\mathbf{A}\mathbf{1})\det([\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]'\mathbf{A}[\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}])= \\ =\delta\det([\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]'\mathbf{A}[\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]). \quad (2.3)$$

By the results of Smaga (to appear), we obtain the following inequality

$$\det([\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]'\mathbf{A}[\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}])\le\Delta(\Delta-4\rho)^2, \quad (2.4)$$

which follows from Hadamard’s inequality and the description of diagonal elements of the matrix $[\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]'\mathbf{A}[\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]$ given in Lemma 2.2 in Katulska and Smaga (2011). Therefore, the inequalities (2.3) and (2.4) imply (2.2). ■

In the following theorem, the lower bound for D-efficiency is given.

Theorem 2.2. Assume that $n\equiv 0 \pmod 4$ and $\rho\in(1/(n-2),1)$. If $\mathbf{X}=[\mathbf{1}\,|\,\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]\in M_{n\times 4}(\pm 1)$, then

$$D-\mathit{eff}\,(\mathbf{X})\ge\left[\frac{\det(\mathbf{X}'\mathbf{A}\mathbf{X})}{\delta\Delta(\Delta-4\rho)^2}\right]^{1/4}. \quad (2.5)$$

Proof. By Lemma 2.1, we obtain

$$\max\{\det(\mathbf{Y}'\mathbf{A}\mathbf{Y}):\mathbf{Y}=[\mathbf{1}\,|\,\mathbf{y}_1\,|\,\mathbf{y}_2\,|\,\mathbf{y}_3]\in M_{n\times 4}(\pm 1)\}\le\delta\Delta(\Delta-4\rho)^2.$$

So, for any arbitrary $\mathbf{X}=[\mathbf{1}\,|\,\mathbf{x}\,|\,\mathbf{y}\,|\,\mathbf{z}]\in M_{n\times 4}(\pm 1)$, it follows that

$$\frac{\det(\mathbf{X}'\mathbf{A}\mathbf{X})}{\max\{\det(\mathbf{Y}'\mathbf{A}\mathbf{Y}):\mathbf{Y}=[\mathbf{1}\,|\,\mathbf{y}_1\,|\,\mathbf{y}_2\,|\,\mathbf{y}_3]\in M_{n\times 4}(\pm 1)\}}\ge\frac{\det(\mathbf{X}'\mathbf{A}\mathbf{X})}{\delta\Delta(\Delta-4\rho)^2}.$$

The function $f(x)=x^{1/4}$ is increasing, therefore from (2.1) we have (2.5). ■

The right hand site of (2.5) is the lower bound for D-efficiency of any biased weighing design with three objects. We denote it by $\underline{D-\mathit{eff}}\,(\mathbf{X})$ for any

$\mathbf{X} = [\mathbf{1} | \mathbf{x} | \mathbf{y} | \mathbf{z}] \in M_{n\times 4}(\pm 1)$. In the next section, we show that the designs $\hat{\mathbf{X}}$ given by (1.2) are highly D-efficient.

3. The D-efficiency of the designs $\hat{\mathbf{X}}$

For the designs $\hat{\mathbf{X}}$ given by (1.2), Katulska and Smaga (2011) proved that

$$\det(\hat{\mathbf{X}}'\mathbf{A}\hat{\mathbf{X}}) = \delta(\Delta - 4\rho)[\Delta(\Delta - 8\rho) - 4\rho^2(1+\rho)^2] + \\ + 4\rho^2(1-\rho)^2(4\rho^2(1+\rho)^2 - \Delta(\Delta - 8\rho)),$$

where δ and Δ are defined in Lemma 2.1. Hence, the following corollary follows immediately from Theorem 2.2.

Corollary 3.1. If $n \equiv 0 \pmod 4$ and $\rho \in (1/(n-2), 1)$, then the lower bound for D-efficiency of the designs $\hat{\mathbf{X}}$ given by (1.2) is of the form

$$\underline{D-eff}(\hat{\mathbf{X}}) =$$

$$= \left[\frac{\delta(\Delta - 4\rho)[\Delta(\Delta - 8\rho) - 4\rho^2(1+\rho)^2] + 4\rho^2(1-\rho)^2(4\rho^2(1+\rho)^2 - \Delta(\Delta - 8\rho))}{\delta\Delta(\Delta - 4\rho)^2}\right]^{1/4},$$

where δ and Δ are given in Lemma 2.1.

We calculated $\underline{D-eff}(\hat{\mathbf{X}})$ for many values of $n \equiv 0 \pmod 4$, $n \geq 8$ and $\rho \in (1/(n-2), 1)$ and we observed that it is very high and in the worst cases it is about 0.94. Moreover, when $n \equiv 0 \pmod 4$, it is easy to see that $\underline{D-eff}(\hat{\mathbf{X}}) = f_n(\rho)$ for all $\rho \in (1/(n-2), 1)$, where the function $f_n : (1/(n-2), 1) \to (0,1)$, is given by $f_n(x) = [L_n(x)/M_n(x)]^{1/4}$ and

$$L_n(x) = -n^2(n-4)^2x^6 - 4n(n-2)(n-4)^2x^5 - (5n^2 - 16n + 16)(n-4)^2x^4 + \\ + 8n(n-4)^2x^3 + n^2(n-4)(5n-12)x^2 + 4n^3(n-4)x + n^4$$

$$M_n(x) = -(n-2)^4 x^6 - 4(n-3)(n-2)^3 x^5 - (5n-18)(n-2)^3 x^4 + \\ + 8n(n-3)(n-2)x^3 + (5n^2 - 24n + 32)n^2 x^2 + 4(n-3)n^3 x + n^4 .$$

Unfortunately, it is difficult to deal with the function f_n analytically. Its properties may be numerically studied. In Figures 1 and 2, the graphs of the function f_n are given for chosen n. From Figures 1 and 2, we observe that the minimum of f_n for $x \in (1/(n-2),1)$ seems to be achieved at some point which is less than one and is not even close to it. In Table 1 and Figure 3, the numerical approximation of the minimum of the function f_n for $x \in (1/(n-2),1)$ is given. Thus, $\min\{f_n(x) : x \in (1/(n-2),1)\}$ is close to one. Therefore, $\underline{D-eff}\,(\hat{\mathbf{X}})$ is greater than or equal to the numerical approximation of $\min\{f_n(x) : x \in (1/(n-2),1)\}$ given in Table 1 and hence the designs $\hat{\mathbf{X}}$ given by (1.2) have high D-efficiency for all $\rho \in (1/(n-2), 1)$.

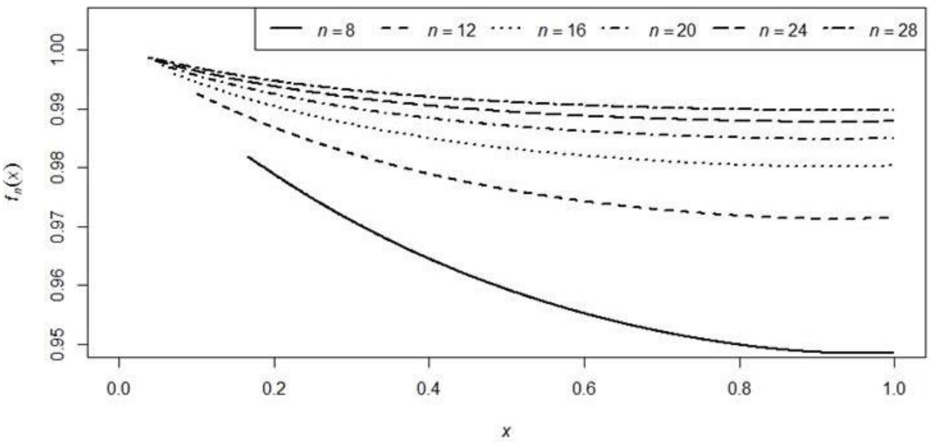

Fig. 1. The graphs of the function f_n for $x \in \left(\frac{1}{n-2}, 1\right)$ and chosen n

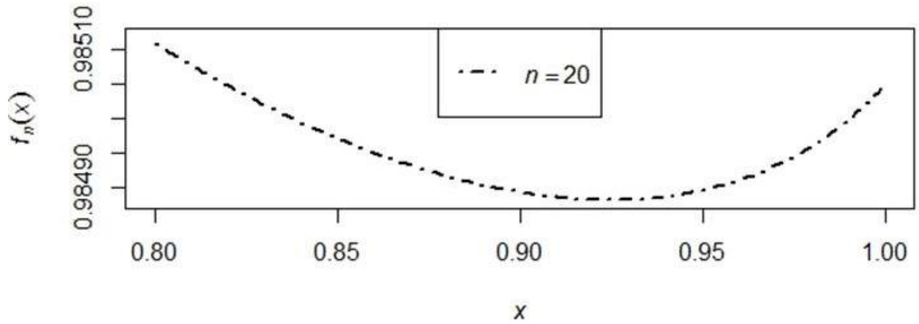

Fig.2. The graph of the function f_n for $x \in (0.8,1)$ and $n = 20$

Table 1. The numerical approximation of $\min\{f_n(x) : x \in (1/(n-2),1)\}$

n	$x_{\min}$	$\min\{f_n(x) : x \in (1/(n-2),1)\}$
8	0.9547769	0.9483788
12	0.9287502	0.9712816
16	0.9242195	0.9801720
20	0.9246333	0.9848817
40	0.9357488	0.9931197
60	0.9446231	0.9955544
80	0.9509150	0.9967180
100	0.9556052	0.9973993

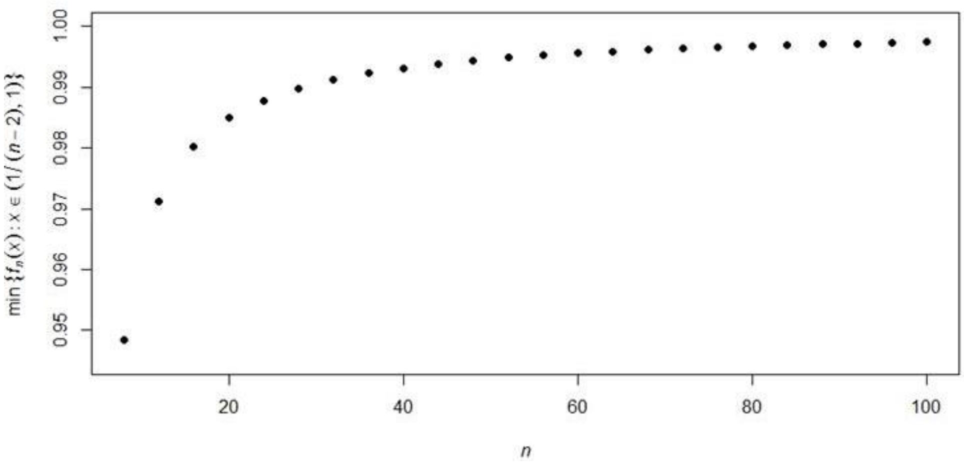

Fig. 3. The numerical approximation of $\min\{f_n(x) : x \in (1/(n-2),1)\}$

4. Conclusions

In this paper, it is shown that the designs constructed by Katulska and Smaga (2011) have high D-efficiency when the D-optimal design is not known in the class of biased chemical balance weighing designs with three objects (i.e., when $\rho \in (1/(n-2), 1)$). This result and simulation study confirm the conjecture that these designs seem to be D-optimal for all $\rho \in [0, 1)$. Unfortunately, it is difficult to prove D-optimality of the considered designs in the model of weighing design with $\mathrm{Var}(\boldsymbol{\varepsilon}) = 1/(1-\rho^2)\mathbf{S}$, where $\mathbf{S} = (\rho^{|r-d|})_{r,d=1}^{n}$. This is the open problem. Nevertheless, the considered designs can be safely used in practice, since the D-efficiency of them is close to one.

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