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Krystyna Katulska; Łukasz Smaga

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D-OPTIMAL AND HIGHLY D-EFFICIENT DESIGNS WITH NON-NEGATIVELY CORRELATED OBSERVATIONS

Krystyna Katulska and Łukasz Smaga

In this paper we consider D-optimal and highly D-efficient chemical balance weighing designs. The errors are assumed to be equally non-negatively correlated and to have equal variances. Some necessary and sufficient conditions under which a design is D*-optimal design (regular D-optimal design) are proved. It is also shown that in many cases D*-optimal design does not exist. In many of those cases the designs constructed by Masaro and Wong (2008) and some new designs are shown to be highly D-efficient. Theoretical results are accompanied by numerical search, suggesting D-optimality of designs under consideration.

Keywords: correlation, D-efficiency, D-optimal chemical balance weighing design, Hadamard matrix, simulated annealing algorithm, tabu search

Classification: 62K05, 15A18

1. INTRODUCTION

Denote by $\mathcal{M}_{n\times p}(S)$ the set of all $n \times p$ matrices with each entry in the set S. First, we present the model of the chemical balance weighing design. Let the observations $y_1, y_2, \ldots, y_n$ follow the linear model $\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{e}$, where $\mathbf{y} = (y_1, \ldots, y_n)'$ is an $n \times 1$ vector of observations, $\mathbf{X}$ is an $n \times p$ design matrix such that $\mathrm{rank}(\mathbf{X}) = p$ ($n \geqslant p$), $\mathbf{b} = (b_1, \ldots, b_p)'$ is a $p \times 1$ vector of unknown parameters, and $\mathbf{e} = (e_1, \ldots, e_n)'$ is an $n \times 1$ vector of errors. Elements of a design matrix $\mathbf{X} = (x_{ij})$ are equal to 1 or -1, i.e. $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1, 1\})$, and $x_{ij} = -1$ or 1 if the jth object is placed on the left or right pan respectively during the ith operation. Moreover, assume that $\mathrm{E}(e_i) = 0$ for all $i = 1, \ldots, n$ and $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\sigma > 0$ is an unknown parameter and $\mathbf{G}$ is an $n \times n$ known positive definite matrix. Since a design matrix is of full column rank, the generalized least-squares estimator of $\mathbf{b}$ equals $\hat{\mathbf{b}} = (\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{G}^{-1}\mathbf{y}$, and its covariance matrix is given by $\sigma^2(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})^{-1}$.

In the class $\mathcal{M}_{n\times p}(\{-1, 1\})$, we would like to choose a design that is the best design with respect to D-optimality criterion. In the literature there are also considered other criteria (see, for example, Pukelsheim [27]), but D-optimality criterion is the most popular. The optimality criteria are expressed in terms of the information matrix of a design $\mathbf{X}$, i.e. a matrix $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}$. We say that $\mathbf{X}$ is D-optimal in $\mathcal{C}$ if it maximizes the determinant of the information matrix among all designs in $\mathcal{C}$. Under certain assumtions on

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the distribution of the error terms, a D-optimal design minimizes the expected volume of the usual confidence ellipsoid for parameters.

An important issue is also the efficiency of a design. Following the definition of Bulutoglu and Ryan [4], the D-efficiency of a design $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$ is

$$\text{D-eff}(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})}{\max_{\mathbf{Y}\in\mathcal{M}_{n\times p}(\{-1,1\})}\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})}\right]^{1/p}.$$

Unfortunately, $\max_{\mathbf{Y}\in\mathcal{M}_{n\times p}(\{-1,1\})}\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})$ is usually not known. However, when an upper bound $\overline{\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})}$ for it is known, D-eff$(\mathbf{X})$ can be approached by a lower bound equal to

$$\text{D}^*\text{-eff}(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})}{\overline{\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})}}\right]^{1/p}. \tag{1}$$

Using (1), we can find designs of high D-efficiency or even D*-optimal designs (i.e. $\det(\mathbf{X}_*'\mathbf{G}^{-1}\mathbf{X}_*) = \overline{\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})}$), since when D*-eff$(\mathbf{X}) = 1$, $\mathbf{X}$ is D*-optimal.

In the literature, optimal and highly efficient designs are considered separately for different forms of the matrix $\mathbf{G}$. It follows from the fact that optimal and highly efficient designs depend significantly on the form of $\mathbf{G}$. Very often, it is assumed that the errors are uncorrelated and they have the same variances. Then, the matrix $\mathbf{G}$ is the identity matrix. For example, Banerjee [2], Ceranka and Graczyk [5], Cheng [9], Ehlich [11, 12], Galil and Kiefer [13], Jacroux et al. [17], Neubauer and Pace [26] (for spring balance) obtained some results about optimal designs under such assumption. In many experimental instances, however, it is quite realistic to assume some sort of dependence (see Angelis et al. [1] for more details, and Jenkins and Chanmugam [18] for real data example). Unfortunately, the case where $\mathbf{G}$ is not the identity matrix, is less explored. When the errors form an AR(1) process, theoretical and numerical search results about A- and D-optimal designs are given in Angelis et al. [1], Bora-Senta and Moyssiadis [3], Katulska and Smaga [20, 21], Li and Yang [24], Smaga [29, 30] and Yeh and Lo Huang [34]. Katulska and Smaga [22], Masaro and Wong [25] and Smaga [29] present some results on the D-optimal designs, when the errors are equally correlated and they have equal variances (the matrix $\mathbf{G}$ is completely symmetric). Ceranka et al. [7], Graczyk [14] and Smaga [29] consider the case where the errors are uncorrelated but may have different variances (the matrix $\mathbf{G}$ is diagonal).

Some applications of weighing designs (in chemistry, medicine, economics, etc.) are given in Angelis et al. [1], Banerjee [2], Cheng [9] and Graczyk [15].

In this paper we consider D-optimal and highly D-efficient designs under the assumption on the matrix $\mathbf{G}$ as in Ceranka and Graczyk [6], Katulska and Smaga [22], Masaro and Wong [25] and Smaga [29, 31]. More precisely, we suppose that

$$\mathbf{G} = (1-\rho)\mathbf{I}_n + \rho\mathbf{1}_n\mathbf{1}_n', \tag{2}$$

where $\rho \in [0,1)$ is a known parameter, $\mathbf{I}_n$ is the $n\times n$ identity matrix, and $\mathbf{1}_n$ is the $n\times 1$ vector of ones. For given ρ, the matrix $\mathbf{G}$ is positive definite and

$$\mathbf{G}^{-1} = c(\mathbf{I}_n - r\mathbf{1}_n\mathbf{1}_n'), \tag{3}$$

where

$$c = \frac{1}{1-\rho}, \quad r = \frac{\rho}{1+(n-1)\rho}. \tag{4}$$

When $n = p$, we have $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) = \det(\mathbf{G}^{-1})\det(\mathbf{X}'\mathbf{X})$, and hence D-optimal design for $\rho = 0$ is also D-optimal for $\rho \neq 0$, so we assume that $n > p$.

The remainder of the present paper is organized as follows. In Section 2, we present necessary and sufficient conditions under which a design is D*-optimal design for $\rho \in [0,1)$ (it means D-optimal design, which satisfies the equality in some inequality for the determinant of the information matrix). We also show that in many cases D*-optimal design does not exist. The lower bound for D-efficiency of weighing designs when $\rho \geqslant 0$ is proved in Section 3. Using that lower bound, we show that some designs constructed by Masaro and Wong [25] and certain new designs are highly D-efficient in many cases where D*-optimal designs do not exist (Sections 3 and 4). Moreover, we also present the best designs found by numerical search in special cases. Finally, Section 5 offers concluding remarks.

2. D*-OPTIMAL DESIGNS FOR $\rho \in [0,1)$

Katulska and Smaga [22] proved the following theorem, which presents the inequality giving the upper bound for the determinant of the information matrix of a design in $\mathcal{M}_{n\times p}(\{-1,1\})$.

Theorem 2.1. (Katulska and Smaga [22]) If $\rho \in [0,1)$, $n \geqslant p+1$, $\mathbf{G}$ is given by the formula (2) and $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$, then

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leqslant \left(\frac{n}{1-\rho}\right)^p. \tag{5}$$

Katulska and Smaga [22] named a design, which satisfies the equality in the inequality (5), as D*-optimal for $\rho \in [0,1)$. Theorem 2.1 implies a D*-optimal design is D-optimal. However, the opposite implication is not true generally, because there are D-optimal designs which are not D*-optimal for some design parameters, i.e. the numbers n, p and ρ (see Theorem 2.3). Katulska and Smaga [22] constructed D*-optimal designs for certain n and p using Hadamard matrices. That construction is also the construction of A-optimal designs considered in Ceranka et al. [8].

In the following theorem, we present some necessary and sufficient conditions under which a design is D*-optimal. They help us to find many values of n and p for which D*-optimal design does not exist. The sufficient conditions were proved in Katulska and Smaga [22].

Theorem 2.2. Let $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$ and $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2).

(*a*) If $\rho \in (0,1)$, then a design $\mathbf{X}$ is D*-optimal if and only if $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$ and $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$, where $\mathbf{0}_p$ is the $p\times 1$ vector of zeros.

(*b*) If $\rho = 0$, then a design $\mathbf{X}$ is D*-optimal if and only if the condition $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$ holds.

P r o o f. The sufficiency follows from Theorem 2.2 in Katulska and Smaga [22]. So, we have to show the necessity. First, we prove (a). Let $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$ be arbitrary. By the Hadamard's inequality, it follows that

$$\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leqslant \prod_{i=1}^{p} \mathbf{x}_i'\mathbf{G}^{-1}\mathbf{x}_i, \tag{6}$$

where $\mathbf{x}_i, i = 1,\ldots,p$, denotes the ith column of $\mathbf{X}$. From (3), we conclude that

$$\mathbf{x}_i'\mathbf{G}^{-1}\mathbf{x}_i = c(\mathbf{x}_i'\mathbf{x}_i - r(\mathbf{x}_i'\mathbf{1}_n)^2) \leqslant cn \tag{7}$$

for all $i = 1,\ldots,p$. So by (6) and (7), we have $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}) \leqslant (cn)^p$. Assume that $\mathbf{X}$ is D*-optimal design. For such design, the equalities must hold in the inequalities (6) and (7). By the condition for equality in Hadamard's inequality, it follows that the equalities in these inequalities imply that the matrix $\mathbf{X}'\mathbf{X}$ is diagonal and $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$. Since $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$, $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$. Point (b), we obtain from the condition for equality in Hadamard's inequality, and the fact that $\mathbf{X}'\mathbf{G}^{-1}\mathbf{X} = \mathbf{X}'\mathbf{X}$ clearly shows that the condition $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$ is not required. □

Theorem 2.3. Assume that $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$, $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2), and $\rho \in (0,1)$. If n is odd, or $n \equiv 2 \pmod 4$ and $p \geqslant 2$, then the D*-optimal design does not exist.

P r o o f. Let n be an odd number. The sum of elements in the ith column of a design matrix $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$ is equal to $n - 2m_i$, $i = 1,\ldots,p$, where m_i is a number of elements of the ith column equal to -1. Hence, since n is odd, the condition $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$ is not satisfied and Theorem 2.2 implies a D*-optimal design does not exist in $\mathcal{M}_{n\times p}(\{-1,1\})$. Suppose now that $n \equiv 2 \pmod 4$ and $p \geqslant 2$. Let p_i be a number of elements of the ith column of $\mathbf{X}$ equal to 1. If there exists i such that p_i is even, then the sum of entries in the ith column of $\mathbf{X}$ is not equal to zero and the condition $\mathbf{X}'\mathbf{1}_n = \mathbf{0}_p$ is not satisfied. Assume now that p_i is odd for all $i = 1,\ldots,p$. Hence, by Lemma 2.2 in Jacroux et al. [17], the absolute value of the inner product of any two columns of $\mathbf{X}$ is greater than or equal to 2. Thus the condition $\mathbf{X}'\mathbf{X} = n\mathbf{I}_p$ is not satisfied. Therefore, Theorem 2.2 implies a D*-optimal design does not also exist when $n \equiv 2 \pmod 4$ and $p \geqslant 2$, so the proof is complete. □

When n is odd, or $n \equiv 2 \pmod 4$ and $p \geqslant 2$, Theorem 2.3 shows that the inequality (5) is useless in finding D-optimal designs in $\mathcal{M}_{n\times p}(\{-1,1\})$. However, it is useful in studying the D-efficiency of designs as we shall see in the next sections.

3. D-EFFICIENT DESIGNS WHEN $N \equiv 1$ (MOD 4)

Assume that $\rho \in [0,1)$. By (5), it follows that $n^p/(1-\rho)^p$ is the upper bound for $\max_{\mathbf{Y}\in\mathcal{M}_{n\times p}(\{-1,1\})} \det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})$. Hence, by (1) and (3), we obtain

$$\text{D}^*\text{-eff}(\mathbf{X}) = \frac{[\det(\mathbf{X}'(\mathbf{I}_n - r\mathbf{1}_n\mathbf{1}_n'))\mathbf{X})]^{1/p}}{n},$$

where r is given in (4), for all $\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\})$. This lower bound for the D-efficiency of the weighing design is a kind of measure which says how far a design is from D*-optimal design. In this section and Section 4, we use it to show that some designs have high D-efficiency in cases where D*-optimal design does not exist.

Let $n \equiv 1 \pmod 4, n \geqslant 5$. Assume that $\mathbf{H}_{n-1} = (\mathbf{1}_{n-1}, \mathbf{h}_1, \ldots, \mathbf{h}_{n-2})$ is an Hadamard matrix of order $n-1$ and $\mathbf{k}_i = (\mathbf{h}_i', 1)'$ for $i = 1, 2, \ldots, n-2$. Masaro and Wong [25] showed that the design $\mathbf{K}$ formed from p columns of $\mathbf{k}_1, \ldots, \mathbf{k}_{n-2}$, is D-optimal for all $\rho > 0$ in the subclass $\mathcal{D}_1 = \{\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1,1\}) : \mathbf{X}'\mathbf{X} = (n-1)\mathbf{I}_p + \mathbf{1}_p\mathbf{1}_p'\}$. Moreover, by the results of Smaga [29], we obtain the following corollary which establishes D-optimality of the designs $\mathbf{K}$ for small number of objects and almost all $\rho \in [0,1)$.

Corollary 3.1. Assume that $n \equiv 1 \pmod 4, n \geqslant p+1$ and $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2). If $p = 2, 3, 4$, then the design $\mathbf{K}$ is D-optimal for ρ belonging to $\{0\} \cup [1/(7n), 1)\,, \{0\} \cup [1/(n+8), 1)\,, \{0\} \cup [1/(n+5), 1)$ respectively.

The proof of this result is long and needs intensive calculation. Its extension for $p \geqslant 5$ seems to be very difficult if possible at all. However, we show that the designs $\mathbf{K}$ are highly D-efficient.

Since $\mathbf{K} \in \mathcal{D}_1$ and $\mathbf{K}'\mathbf{1}_n = \mathbf{1}_p$, $\mathbf{K}'(\mathbf{I}_n - r\mathbf{1}_n\mathbf{1}_n')\mathbf{K}$ has eigenvalues $n-1$ and $n-1+(1-r)p$ with multiplicities $p-1$ and 1 respectively. So, for the design $\mathbf{K}$ we have

$$\mathrm{D}^*\text{-eff}(\mathbf{K}) = \frac{n-1}{n}\left[\frac{n+p-1-pr}{n-1}\right]^{1/p}, \tag{8}$$

where r is given in (4).

Theorem 3.2. Let $n \equiv 1 \pmod 4, n \geqslant 5, p = 2, \ldots, n-2, \rho \in (0,1)$ and $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2). Then, $\mathrm{D}^*\text{-eff}(\mathbf{K})$ decreases, when ρ increases. Moreover, $\mathrm{D}^*\text{-eff}(\mathbf{K})$ is greater than 0.93.

P r o o f. Since r is an increasing function of ρ, it is easy to see that $\mathrm{D}^*\text{-eff}(\mathbf{K})$ decreases, when ρ increases. Hence, $\mathrm{D}^*\text{-eff}(\mathbf{K})$ is greater than the right hand side of (8) for $\rho = 1$, i.e. $((n-1)/n)[(n+p)/n]^{1/p}$. Consider the function $f, f : (1, n-1) \to \mathbb{R}$ given by $f(x) = [(n+x)/n]^{1/x}$. Its derivative is equal to $[(n+x)/n]^{1/x}x(1-(1+n/x)\log(1+x/n))/(x^2(n+x))$, where log denotes the natural logarithm. Suppose $g, g : (1, \infty) \to \mathbb{R}$ is the function defined by $g(x) = 1-(1+x)\log(1+1/x)$. Using l'Hospital's rule, it is easy to show that $\lim_{x\to\infty} g(x) = 0$. Moreover, we have $g'(x) = 1/x - \log(1+1/x)$, $g'(x) \to 0$ as $x \to \infty$ and $g''(x) = -1/(x^3+x^2)$. Therefore, $g'(x) > 0$ and hence g is an increasing function. Since g is increasing and $g(x) \to 0$ as $x \to \infty$, $g(x)$ is negative for all $x > 1$. But $n/x > 0$ for all $x \in (1, n-1)$, so $f'(x) < 0$. Thus

$$\mathrm{D}^*\text{-eff}(\mathbf{K}) > ((n-1)/n)f(n-2) = ((n-1)/n)[2(n-1)/n]^{1/(n-2)}. \tag{9}$$

Consider the function $h, h : (8, \infty) \to \mathbb{R}$, which is given by the formula $h(x) = ((x-1)/x)[2(x-1)/x]^{1/(x-2)}$. The derivative of h equals

$$h'(x) = \frac{[2(x-1)/x]^{1/(x-2)}(x-1)(x\log(x/(x-1)) + x(1-\log(2)) - 2)}{(x-2)^2x^2}$$

and it is positive, since $x > 8$. Hence, h is increasing. From (9), it follows that $\text{D}^*\text{-eff}(\mathbf{K}) > \min\{h(5), h(9)\} = 0.9356$. The proof is complete. $\square$

Let us see on examples how $\text{D}^*\text{-eff}(\mathbf{K})$ behaves. Theorem 3.2 shows that $\text{D}^*\text{-eff}(\mathbf{K})$ decreases as ρ increases. However, the examples suggest that the decrease of $\text{D}^*\text{-eff}(\mathbf{K})$ is not significant in this case and it decreases, when p or n increases (see, for example, Table 1). Unfortunately, the decrease of $\text{D}^*\text{-eff}(\mathbf{K})$ can be greater as p increases, but the decrease of the lower bound for the D-efficiency of $\mathbf{K}$ decreases as n increases, which we see in Table 2. Fortunately, from Table 3, we conclude that $\text{D}^*\text{-eff}(\mathbf{K})$ increases quite fast as n increases. In Tables 2 and 3 the values of $\text{D}^*\text{-eff}(\mathbf{K})$ were calculated for $\rho = 0.99$. Since $\text{D}^*\text{-eff}(\mathbf{K})$ decreases as ρ increases, this value of ρ is "the worst" for $\text{D}^*\text{-eff}(\mathbf{K})$. So, for the same values of n and p, the $\text{D}^*\text{-eff}(\mathbf{K})$ is greater for smaller values of ρ. In Theorem 3.2, we proved the lower bound for $\text{D}^*\text{-eff}(\mathbf{K})$, but from examples we see that it is much greater than that lower bound in many cases.

ρ	$\text{D}^*\text{-eff}(\mathbf{K})$	$\text{D}^*\text{-eff}(\mathbf{K})$	$\text{D}^*\text{-eff}(\mathbf{Z})$	$\text{D}^*\text{-eff}(\mathbf{Z})$
0	0.9938	0.9724	1.0000	0.9567
0.01	0.9928	0.9718	0.9981	0.9557
0.1	0.9882	0.9687	0.9894	0.9504
0.2	0.9861	0.9673	0.9856	0.9481
0.3	0.9850	0.9665	0.9836	0.9469
0.4	0.9842	0.9661	0.9824	0.9462
0.5	0.9838	0.9657	0.9816	0.9457
0.6	0.9834	0.9655	0.9810	0.9454
0.7	0.9832	0.9653	0.9806	0.9451
0.8	0.9830	0.9652	0.9802	0.9449
0.9	0.9828	0.9651	0.9800	0.9447
0.99	0.9827	0.9650	0.9798	0.9446
n, p	$9, 2$	$9, 7$	$10, 2$	$10, 7$

Tab. 1. The lower bound for D-efficiency of designs $\mathbf{K}$ and $\mathbf{Z}$.

To show more clearly that the design $\mathbf{K}$ is a very good design under criterion of D-optimality, we compared it with the best designs found by simulated annealing algorithm (SA algorithm) from Angelis et al. [1] and by tabu-search-based approach (see, for example, Harman et al. [16], Jung and Yum [19]). SA and tabu-search algorithms are algorithms for searching optimal designs with very good performance, so we use them to find D-efficient designs in $\mathcal{M}_{n\times p}(\{-1, 1\})$ with $\text{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2). We chose $T_0 = 1$, $I = 25$ and $R = 0.95$, or even greater values of I and R in some cases, as the initial parameters of SA algorithm, since these are right choices by the results of Angelis et al. [1]. When $T_0 = 1$, $I = 25$ and $R = 0.95$, the SA algorithm was executed at least 5000 times for many values of the design parameters namely n, p and ρ. Generally, larger values of I and R (for example $I = 100$, $R = 0.99$) have a beneficial effect on the performance of the algorithm, but they increase dramatically the duration of the search, so we executed SA algorithm for such I and R less times than

p	D*-eff(**K**)	D*-eff(**K**)	D*-eff(**Z**)	D*-eff(**Z**)
1	0.9600	0.9965	1.0000	1.0000
2	0.9466	0.9950	0.9429	0.9938
3	0.9357	0.9935	0.9245	0.9917
4		0.9922		0.9882
5		0.9909		0.9861
6		0.9898		0.9833
7		0.9887		0.9814
8		0.9876		0.9790
9		0.9866		0.9772
10		0.9857		0.9752
11		0.9848		0.9736
12		0.9840		0.9718
13		0.9832		0.9703
14		0.9824		0.9687
15		0.9817		0.9673
n	5	17	6	18

Tab. 2. The lower bound for D-efficiency of designs **K** and **Z** ($\rho = 0.99$).

n	D*-eff(**K**)	n	D*-eff(**Z**)
21	0.9852	22	0.9730
25	0.9889	26	0.9797
29	0.9914	30	0.9842
33	0.9931	34	0.9873
37	0.9944	38	0.9896
41	0.9953	42	0.9913

Tab. 3. The lower bound for D-efficiency of designs **K** and **Z** ($p = 19, \rho = 0.99$).

when $I = 25$ and $R = 0.95$. In a tabu-search-based approach, the number of iterations in the preliminary search of the algorithm was chosen to be equal to 150 (usually) or 250 (for more difficult cases). A number of neighbour designs to check at each iteration was np. The tabu-search algorithm was executed 1000 times for the same values of the design parameters as for SA algorithm. In the present framework, the tabu-search-based approach may be easily implemented in the R program [28] (see Appendix). What is very interesting and important, the SA and tabu-search algorithms did not find D-better designs than the design **K**. Moreover, the tabu-search found the design **K** as the best design under D-optimality criterion. For smaller values of p, the SA algorithm did the same, but for greater values of p (especially for p near to n) it found designs with the lower bound for D-efficiency clearly lower than D*-eff(**K**). As an example, we present in

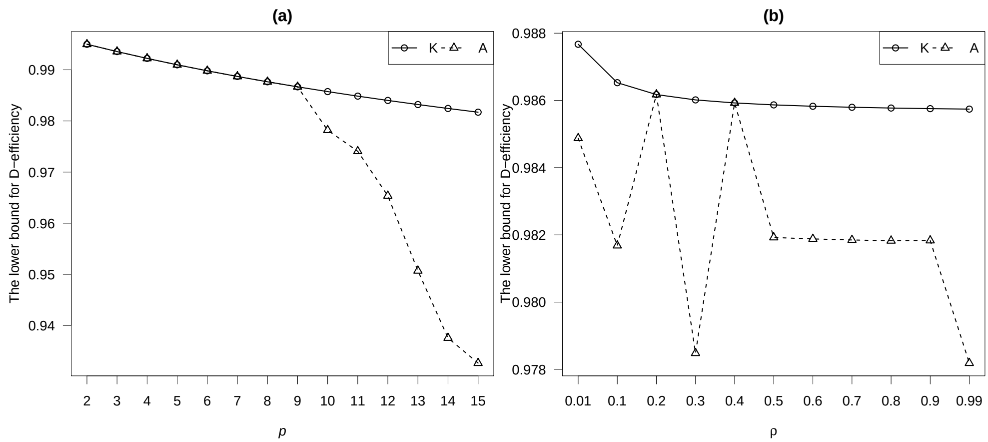

Fig. 1. The lower bound for D-efficiency of design $\mathbf{K}$ (K) and the best designs found by the SA algorithm (A) for **(a)** $n = 17$ and $\rho = 0.99$, **(b)** $n = 17$ and $p = 10$. The lower bound for D-efficiency the best designs found by the tabu-search algorithm equals to that of $\mathbf{K}$.

Figure 1 (a) the lower bound for D-efficiency of design $\mathbf{K}$ and the best designs found by SA algorithm ($T_0 = 1$, $I = 25$ and $R = 0.95$) for $n = 17$, $p = 2, \ldots, 15$, and $\rho = 0.99$. For fixed n and p, the SA algorithm behave quite stable for different values of ρ. However, for some ρ, it found $\mathbf{K}$ as the best design, but for the other it did not do that (see Figure 1 (b)). So, the SA algorithm perform quite well, but not better than the design $\mathbf{K}$ and the tabu-search algorithm.

To summarize theoretical (see, Corollary 3.1 and Theorem 3.2) and numerical search results, we can conclude that the design $\mathbf{K}$ is a design with high D-efficiency and it seems to be D-optimal for all $\rho \in (0, 1)$, when it exists.

Ehlich [11] showed that an $\mathbf{X} \in \mathcal{M}_{n\times n}(\{-1, 1\})$ with $\mathbf{X}'\mathbf{X} = (n-1)\mathbf{I}_n + \mathbf{1}_n\mathbf{1}_n'$ is D-optimal for $\rho = 0$ and as we noticed in Section 1 it is also D-optimal for $\rho \neq 0$. Such designs can exist only if $2n-1$ is the square of an integer and they are known for example for "practical" values $n = 5, 13, 25$. We now take into consideration the near-saturated case $p = n-1$ and $\rho \geqslant 0$. One can negate every row of $\mathbf{X} \in \mathcal{M}_{n\times n}(\{-1, 1\})$ with $\mathbf{X}'\mathbf{X} = (n-1)\mathbf{I}_n + \mathbf{1}_n\mathbf{1}_n'$, whose first element equals -1, and hence $\mathbf{X} = (\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_{n-1})$. So, the design $\mathbf{N} = (\mathbf{x}_1, \ldots, \mathbf{x}_{n-1})$ has the following properties $\mathbf{N}'\mathbf{N} = (n-1)\mathbf{I}_{n-1} + \mathbf{1}_{n-1}\mathbf{1}_{n-1}'$ and $\mathbf{N}'\mathbf{1}_n = \mathbf{1}_{n-1}'$, similarly as the design $\mathbf{K}$. Therefore, D*-eff$(\mathbf{N}) = ((n-1)/n)(2-r)^{1/(n-1)}$ and it is greater than 0.92. Thus, if $p = n-1$, $\rho \in (0, 1)$ and the design $\mathbf{N}$ exists, then it is highly D-efficient and we did not find (in numerical search) D-better design than it. In some cases where $\mathbf{N}$ does not exist, the webpage `http://www.staff.amu.edu.pl/~ls/str_en.html` lists the best designs under D-optimality criterion found by SA and tabu-search algorithms. We observe that the inner product of any two columns of these designs is equal to ± 1, and the sum of elements in any column equals ± 1 or ± 3 (for the vast majority of columns) or less frequently ± 5.

4. D-EFFICIENT DESIGNS WHEN $N \equiv 2$ (MOD 4)

In this section, we shortly consider the case where $n \equiv 2 \pmod 4$, since it is similar to the previous. Assume that $\mathbf{H}_{n-2} = (\mathbf{1}_{n-2}, \mathbf{h}_1, \ldots, \mathbf{h}_{n-3})$ is an Hadamard matrix of order $n-2$. Then, we define the designs $\mathbf{Z} = (\mathbf{z}_1, \ldots, \mathbf{z}_p)$, where $\mathbf{z}_i = (\mathbf{h}_i', 1, -1)'$ for $i = 1, \ldots, s$, $\mathbf{z}_j = (\mathbf{h}_j', 1, 1)'$ for $j = s+1, \ldots, p$, and $s = [(p+1)/2]$ ($[x]$ is the integral part of x). Such designs may exist for $p \leqslant n-3$. Masaro and Wong [25] proved that the designs $\mathbf{Z}$ are D-optimal for all $\rho > 0$ in the subclass

$$\mathcal{D}_2 = \{\mathbf{X} : \mathbf{X}'\mathbf{X} = \operatorname{diag}\left[(n-2)\mathbf{I}_s + 2\mathbf{1}_s\mathbf{1}_s', (n-2)\mathbf{I}_{p-s} + 2\mathbf{1}_{p-s}\mathbf{1}_{p-s}'\right]\}.$$

Furthermore, the following result shows that the designs $\mathbf{Z}$ are D-optimal for $p = 2, 3, 4$ and almost all $\rho \in [0, 1)$. It is a consequence of the results of Smaga [29].

Corollary 4.1. Suppose that $n \equiv 2 \pmod 4), n \geqslant p+1$ and $\operatorname{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2). If $p = 2, 3, 4$, then the design $\mathbf{Z}$ is D-optimal for ρ belonging to $[0, 1)$, $\{0\} \cup (1/(3n+1), 1)$, $\{0\} \cup (1/(n+6), 1)$ respectively.

Similarly as for the case $n \equiv 1 \pmod 4$, it seems that it is difficult to extend this corollary for greater number of objects. Therefore, we once again investigate D-efficiency of the designs $\mathbf{Z}$.

It is easy to see that $\mathbf{z}_i'\mathbf{1}_n = 0$ for $i = 1, \ldots, s$, and $\mathbf{z}_j'\mathbf{1}_n = 2$ for $j = s+1, \ldots, p$. If p is odd, then $\mathbf{Z}'(\mathbf{I}_n - r\mathbf{1}_n\mathbf{1}_n')\mathbf{Z}$ has eigenvalues $n-2$, $n+p-1$ and $n-2+(1-2r)(p-1)$ with multiplicities $p-2, 1$ and 1 respectively. When p is even, $\mathbf{Z}'(\mathbf{I}_n - r\mathbf{1}_n\mathbf{1}_n')\mathbf{Z}$ has eigenvalues $n-2$, $n+p-2$ and $n-2+(1-2r)p$ with multiplicities $p-2, 1$ and 1 respectively. So, we have

$$\text{D}^*\text{-eff}(\mathbf{Z}) = \begin{cases} \frac{n-2}{n}\left[\frac{(n+p-1)(n-2+(1-2r)(p-1))}{(n-2)^2}\right]^{1/p} & \text{if } p \text{ is odd}, \\ \frac{n-2}{n}\left[\frac{(n+p-2)(n-2+(1-2r)p)}{(n-2)^2}\right]^{1/p} & \text{if } p \text{ is even}, \end{cases} \tag{10}$$

where r is given in (4). So, we consider two cases: p is odd or even. In both these cases, the results for the lower bound for D-efficiency of the designs $\mathbf{Z}$ are very similar to those for D*-eff$(\mathbf{K})$ (see, Theorem 4.2 and Tables 1-3), so we do not discuss them in detail. The designs $\mathbf{Z}$ are also highly D-efficient designs and seem to be D-optimal for all $\rho > 0$ in those cases where they exist.

Theorem 4.2. Let $n \equiv 2 \pmod 4), n \geqslant 6$, $\rho \in (0, 1)$ and $\operatorname{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (2).

(*a*) If $p = 3, 5, \ldots, n-3$, then D*-eff$(\mathbf{Z})$ decreases, when ρ increases, and D*-eff$(\mathbf{Z})$ is greater than 0.92.

(*b*) If $p = 2, 4, \ldots, n-4$, then D*-eff$(\mathbf{Z})$ decreases, when ρ increases and D*-eff$(\mathbf{Z}) > 0.94$.

P r o o f. First, we present the proof of part (*a*). It is easy to see that D*-eff$(\mathbf{Z})$ decreases, when ρ increases. Hence

$$\text{D}^*\text{-eff}(\mathbf{Z}) > \frac{n-2}{n}\left[\frac{(n+p-1)(n-2+(1-2/n)(p-1))}{(n-2)^2}\right]^{1/p}$$

(the right hand side of (10) for $\rho = 1$). We define the function $f, f : (2, n-2) \to \mathbb{R}$ by

$$f(x) = \left[\frac{(n+x-1)(n-2+(1-2/n)(x-1))}{(n-2)^2} \right]^{1/x}.$$

We have

$$f'(x) = \frac{[(n+x-1)^2/((n-2)n)]^{1/x} m(n,x)}{x^2(n+x-1)},$$

where $m(n,x) = 2x - (n+x-1)\log((n+x-1)^2/((n-2)n))$. Direct calculations show that $m(n,x) = 2(x-1)g(n/(x-1)) - x\log(n/(n-2)) + k(n)$, where g is defined in the proof of Theorem 3.2, and $k, k : (5, \infty) \to \mathbb{R}$ is the function given by $k(x) = 2 - (x-1)\log(x/(x-2))$. From the proof of Theorem 3.2, it follows that $g(n/(x-1)) < 0$. We have $k'(x) = 2(x-1)/(x(x-2)) - \log(x/(x-2)) \to 0$ as $x \to \infty$, and $k''(x) = -4/((x-2)^2x^2) < 0$. Hence $k'(x) > 0$ and k is increasing. Using l'Hospital's rule, we can show that $\lim_{x\to\infty} k(x) = 0$. Thus, $k(x) < 0$ for all $x > 5$ and hence $f'(x) < 0$. So, f is decreasing, which implies D*-eff$(\mathbf{Z}) > ((n-2)/n)f(n-3) = ((n-2)/n)[4(n-2)/n]^{1/(n-3)}$. Consider the function $h, h : (5.9, \infty) \to \mathbb{R}$ given by $h(x) = ((x-2)/x)[4(x-2)/x]^{1/(x-3)}$. Its derivative equals

$$h'(x) = -\frac{[4(x-2)/x]^{1/(x-3)}(x-2)(6-2x+x\log(4(x-2)/x))}{(x-3)^2x^2}.$$

If $h_1(x) = 6-2x+x\log(4(x-2)/x)$, then $h_1'(x) = (6-2x+(x-2)\log(4(x-2)/x))/(x-2)$ and $h_1''(x) = -4/((x-2)^2x) < 0$. Since $h_1'(5.9) < 0$, we conclude that $h_1'(x) < 0$. So, $h_1(x) < 0$, because $h_1(5.9)$ is negative. Therefore, h is an increasing function, which implies D*-eff$(\mathbf{Z}) > h(6) = 0.9245$.

Now, we prove the part (b). Since D*-eff$(\mathbf{Z})$ decreases, when ρ increases and by (10), the inequality

$$\text{D}^*\text{-eff}(\mathbf{Z}) > \frac{n-2}{n}\left[\frac{(n+p-2)(n-2+(1-2/n)p)}{(n-2)^2}\right]^{1/p}$$

holds. Set

$$f(x) = \frac{x-2}{x}\left[\frac{(x+p-2)(x-2+(1-2/x)p)}{(x-2)^2}\right]^{1/p}$$

for all $x \in (p+3, \infty)$. We have

$$f'(x) = 2\left[\frac{(x+p-2)(x+p)}{x(x-2)}\right]^{1/p-1}\frac{(x-1)p+p^2-2}{(x-2)x^3} > 0.$$

So, D*-eff$(\mathbf{Z}) > f(p+4) = ((p+2)/(p+4))[4(p+1)/(p+4)]^{1/p}$. Consider the function $l, l : (1, \infty) \to \mathbb{R}$ given by $l(x) = ((x+2)/(x+4))[4(x+1)/(x+4)]^{1/x}$. It can be calculated that $l(2) = 0.9428$, $l(4) = 0.9431$, $l(6) = 0.9498$, $l(8) = 0.956$, $l(10) = 0.9611$ and $l(12) = 0.9653$. The derivative of l is of the form

$$l'(x) = \frac{4^{1/x}[(x+1)/(x+4)]^{1/x-1}k(x)}{x^2(x+4)^3},$$

where $k(x) = x(2x^2 + 5x + 6) - (x^3 + 7x^2 + 14x + 8)\log(4(x + 1)/(x + 4))$. Since $\log(4(x+1)/(x+4)) < \log(4)$, $l'(x)$ is greater than

$$\frac{4^{1/x}[(x+1)/(x+4)]^{1/x-1}h(x)}{x^2(x+4)^3},$$

where $h(x) = x(2x^2 + 5x + 6) - \log(4)(x^3 + 7x^2 + 14x + 8)$. We have $h'(x) = 3(2 - \log(4))x^2 - 2(7\log(4) - 5)x + 6 - 14\log(4) > 0$ for all $x > 11$. Hence h is increasing for all $x > 11$ and since $h(11) > 0$, we obtain $h(x) > 0$ for $x > 11$. Therefore, $l'(x) > 0$ and l is increasing for $x > 11$. Summarizing, $\text{D}^*\text{-eff}(\mathbf{Z}) > l(2) > 0.94$. □

In cases $p = n - 1$ and $p = n - 2$, we can sometimes construct highly D-efficient designs from some D-optimal design in $\mathcal{M}_{n\times n}(\{-1, 1\})$. Ehlich [11] and Wojtas [32] showed that an $\mathbf{X} \in \mathcal{D}_2 \subseteq \mathcal{M}_{n\times n}(\{-1, 1\})$ with $s = n/2$ is D-optimal in $\mathcal{M}_{n\times n}(\{-1, 1\})$. Such designs can be constructed in all cases $n \leqslant 54$ except $n = 22$ and 34 (see Yang [33]). We can negate every row of $\mathbf{X}$, whose last element is equal to -1. Then, $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_{n-1}, \mathbf{1}_n)$. The designs $\mathbf{X}_k = (\mathbf{x}_k, \ldots, \mathbf{x}_{n-1})$ for $k = 1, 2$ belong to $\mathcal{D}_2$ with $s = n/2, n/2 - 1$, respectively, and $\mathbf{x}_i'\mathbf{1}_n = 0$ for $i = 1, \ldots, n/2$, and $\mathbf{x}_i'\mathbf{1}_n = 2$ for $i = n/2 + 1, \ldots, n - 1$, similarly as the designs $\mathbf{Z}$. Hence, we have

$$\text{D}^*\text{-eff}(\mathbf{X}_k) = \begin{cases} \frac{n-2}{n}\left[4(1-r)\right]^{1/(n-2)} & \text{if } k = 2 \\ \frac{n-2}{n}\left[\frac{4(n-1)(1-r)}{n-2}\right]^{1/(n-1)} & \text{if } k = 1. \end{cases}$$

The inequalities $\text{D}^*\text{-eff}(\mathbf{X}_2) > 0.9$ and $\text{D}^*\text{-eff}(\mathbf{X}_1) > 0.88$ hold. Therefore, the designs $\mathbf{X}_k$ for $k = 1, 2$ are highly D-efficient when $\rho \in (0, 1)$ and $p = n - 1, n - 2$, respectively, and we did not find (in numerical search) D-better designs than them in some cases of their existence. Some examples of such designs found by SA and tabu-search algorithms are also reported on the webpage mentioned above.

5. CONCLUSIONS

In this paper we established the situations where D*-optimal designs considered in Katulska and Smaga [22] do not exist. In many of those situations, namely when $n \equiv 1,\ 2 \pmod 4$, we showed that the designs constructed by Masaro and Wong [25] and some new designs are highly D-efficient. Numerical search conducted did not find D-better designs than those. Therefore, the designs constructed by Masaro and Wong [25] may be used safely in practice when the number of observations $n \equiv 1,\ 2 \pmod 4$. The situation changes in the most difficult case where $n \equiv 3 \pmod 4$. It has recently been obtained by Katulska and Smaga [23] that in this case, the designs constructed by Masaro and Wong [25] seem to be D-optimal when the number of observations is appropriately large or appropriately larger than the number of objects. In the other cases, however, D-better designs exist.

APPENDIX

R code for a tabu-search-based approach

A tabu-search-based approach for D-efficient designs is performed by the following R code. We use the function `tabuSearch` from the R package `tabuSearch` (Domijan [10]). This function performs a tabu-search algorithm for optimizing binary strings. The parameters of a design, namely the number of observations n, the number of objects p and the value of parameter ρ, need to be fixed. For instance, in the following code, we have $n = 5$, $p = 4$ and $\rho = 0.7$. The number of iterations in the preliminary search of the algorithm is 150 (the argument `iters` in the function `tabuSearch`) and the number of times to repeat the search is 1000 (the argument `repeatAll` in the function `tabuSearch`). As a result, we obtain the best design found by tabu-search algorithm under D-optimality criterion and its D-efficiency.

```
# parameters of a design
n = 5; p = 4; rho = 0.7

# the constant defined in (4)
r = rho/(1+(n-1)*rho)

# the objective function
det.max = function(x){
  x[x == 0] = -1
  temp = matrix(x, nrow = n, ncol = p)
  sums = t(colSums(temp))
  return(det(t(temp) %*% temp - r * t(sums) %*% sums))
}

# performing of a tabu-search algorithm
library(tabuSearch)
res = tabuSearch(size = n*p, iters = 150, objFunc = det.max,
                 repeatAll = 1000)

# the maximal D-efficiency obtained
max.D.eff = (max(res$eUtilityKeep)^(1/p))/n

# the best design obtained under D-optimality criterion
D.best.string = (res$configKeep)[which.max(res$eUtilityKeep),]
D.best.string[D.best.string == 0] = -1
D.best.design = matrix(D.best.string, nrow = n, ncol = p)
```

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Krystyna Katulska, Faculty of Mathematics and Computer Science, Adam Mickiewicz University, Umultowska 87, 61-614 Poznań. Poland.
e-mail: krakat@amu.edu.pl

Łukasz Smaga, Faculty of Mathematics and Computer Science, Adam Mickiewicz University, Umultowska 87, 61-614 Poznań. Poland.
e-mail: ls@amu.edu.pl