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CRITERION-ROBUST DESIGNS FOR THE MODELS OF SPRING BALANCE WEIGHING

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ABSTRACT. In the paper we consider the linear regression model of the first degree on the vertices of the d-dimensional unit cube and its extension by an intercept term, which can be used, e.g., to model unbiased or biased weighing of d objects on a spring balance. In both settings, we can restrict our search for approximate optimal designs to the convex combinations of the so-called j-vertex designs. We focus on the designs that are criterion robust in the sense of maximin efficiency within the class of all orthogonally invariant information functions, involving the criteria of D-, A-, E-optimality, and many others. For the model of unbiased weighing, we give analytic formulas for the maximin efficient design, and for the biased model we present numerical results based on the application of the methods of semidefinite programming.

1. Introduction

Consider the linear regression model of the first degree on the vertices of the d-dimensional unit cube given by the formula

$$y = x_1\beta_1 + \cdots + x_d\beta_d + \varepsilon, \tag{1}$$

where y is a real-valued observation, $\beta_1, \ldots, \beta_d$ are unknown parameters, $x_1, \ldots, x_d \in \{0, 1\}$, and ε is a random error with zero mean. A possible interpretation of the model is that $\beta_1, \ldots, \beta_d$ represent unknown weights of d items, and $x_1, \ldots, x_d$ mean the presence or the absence of the items in a weighing by a spring balance. The experimental design for this model is a rule for selecting the items present in different weighings, with the aim to obtain a good estimator of the unknown weights.

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Besides the classical model (1), we will focus on its extension by an intercept term

$$y = x_1\beta_1 + \cdots + x_d\beta_d + c\beta_{d+1} + \varepsilon. \tag{2}$$

In the weighing interpretation, β_{d+1} can represent an unknown constant bias of the spring balance caused, e.g., by an additional item that is necessarily present in all the weighings. The constant c is usually chosen to be 1, but selecting different values of c allows us to change the relative importance of the estimation of the bias term compared to the estimation of the parameters representing weights of the objects. For details, see the paper [6].

Jacroux and Notz [9] analyzed the optimality of the spring balance weighing designs without a constant bias for a large class of criteria depending on the eigenvalues of the information matrix, and Cheng [2] used the Kiefer-Wolfowitz theorem to find all approximate Φ_p-optimal designs. Next, Pukelsheim [11] determined a complete class of designs for this model, and Dette and Studden [4] described a geometric construction of approximate E-optimal designs. From the optimal design perspective, the model (2) with a constant bias was analyzed in the paper [6]. In some cases, the model (2) with $c = 1$ admits exact designs that lead to the minimum achievable variance of the estimators of the weights, which was shown in [1].

Next, we will introduce the basic concepts from the point of view of general linear regression models; for details, see the monographs [10] and [11].

Consider a linear regression model on a compact experimental domain $\mathfrak{X} \subseteq \mathbb{R}^s$. For each design point $x \in \mathfrak{X}$ we can observe a real-valued random variable $y = f^T(x)\beta + \varepsilon$, where $f : \mathfrak{X} \to \mathbb{R}^m$ is a vector of known continuous regression functions, $\beta \in \mathbb{R}^m$ is a vector of unknown parameters, and ε is a random error with $\mathrm{E}(\varepsilon) = 0$. For different observations, the errors are assumed to be uncorrelated with a constant variance. We will denote this model by $(f, \mathfrak{X})$ and say that the model is m-parametric.

For the models (1) and (2), the experimental domain is $\mathfrak{X} = \{0, 1\}^d$, and the vectors of regression functions are the identity mapping and

$$f : \mathfrak{X} \to \mathbb{R}^{d+1}; \quad f(x_1, \ldots, x_d) = (x_1, \ldots, x_d, c)^T,$$

respectively. Likewise, $m = d$ in the model (1) and $m = d + 1$ in the model (2).

An (approximate) experimental design is a probability measure ξ on $\mathfrak{X}$ with a finite support. Note that for the weighing models, the experimental domain $\mathfrak{X}$ is finite, that is, any probability measure on $\mathfrak{X}$ is a design. The value $\xi(x)$ represents the relative frequency of replications to be taken in x. By Ξ we denote the set of all designs on $\mathfrak{X}$. The performance of a design $\xi \in \Xi$ is based on the information matrix

$$\mathbf{M}(\xi) = \sum_{x \in \mathfrak{X}} f(x) f^T(x) \xi(x).$$

An optimality criterion Φ is a real-valued function defined on the set of information matrices, measuring the quality of the corresponding design. A design ξ^* is said to be Φ-optimal if

$$\Phi\big(\mathbf{M}(\xi^*)\big) = \sup_{\xi\in\Xi} \Phi\big(\mathbf{M}(\xi)\big). \tag{3}$$

If (3) holds, then $\mathbf{M}(\xi^*)$ is called a Φ-optimal information matrix, and $\Phi\big(\mathbf{M}(\xi^*)\big)$ is called the Φ-optimal value of the model $(f, \mathfrak{X})$. The quality of a design ξ compared to a Φ-optimal design ξ^* is measured by its Φ-efficiency

$$\mathrm{eff}(\xi \mid \Phi) = \frac{\Phi(\mathbf{M}(\xi))}{\Phi(\mathbf{M}(\xi^*))}. \tag{4}$$

Let Φ_{E_k}, $k = 1, \ldots, m$, be the so-called E_k-criteria of optimality introduced in [7], that is, $\Phi_{E_k} : \mathcal{S}_+^m \to [0, \infty)$ is defined as the sum of k smallest eigenvalues of the matrix

$$\Phi_{E_k}(\mathbf{M}) = \sum_{i=1}^{k} \lambda_i(\mathbf{M}).$$

The symbol $\mathcal{S}_+^m$ denotes the set of symmetric nonnegative definite matrices of type $m \times m$ and $\lambda(\mathbf{M})$ denotes the vector of all eigenvalues of $\mathbf{M} \in \mathcal{S}_+^m$ arranged in nondecreasing order.

Let $\mathbb{O}$ denote the class of all orthogonally invariant criteria, i.e., all information functions of the type $\Phi : \mathcal{S}_+^m \to [0, \infty)$ that satisfy the condition of orthogonal invariance

$$\Phi(\mathbf{U}\mathbf{C}\mathbf{U}^T) = \Phi(\mathbf{C})$$

for all $\mathbf{C} \in \mathcal{S}_+^m$ and $m \times m$ orthogonal matrices $\mathbf{U}$ (see [11] and [7]). Note that for any information function Φ, there exists a Φ-optimal design, and the criterion Φ is positively homogeneous, which justifies the particular definition of design efficiency given by equation (4). The class $\mathbb{O}$ contains concave and positively homogeneous versions of essentially all reasonable optimality criteria that depend only on the eigenvalues of the information matrix, such as the criteria of E-, E_k-, D-, A-optimality and many others. It turns out that the minimal efficiency of a design ξ with respect to the whole class $\mathbb{O}$, i.e., a stability of performance of ξ with respect to a very broad class of criteria, can be calculated using the criteria of E_k-optimality (see [7])

$$\begin{aligned} \mathrm{mineff}(\xi|\mathbb{O}) &:= \min_{\Phi\in\mathbb{O}} \mathrm{eff}(\xi \mid \Phi) \\ &= \min_{k=1,\ldots,m} \mathrm{eff}(\xi \mid \Phi_{E_k}) \\ &= \min_{k=1,\ldots,m} \frac{\Phi_{E_k}(\mathbf{M}(\xi))}{v(k)}, \end{aligned} \tag{5}$$

where $v(k)$ denotes the Φ_{E_k}-optimal value (or, for brevity, the E_k-optimal value). The number $\operatorname{mineff}(\xi|\mathbb{O})$ will be called the $\mathbb{O}$-minimal efficiency of the design ξ for the model $(f, \mathfrak{X})$, or, briefly, the minimal efficiency of ξ.

Knowing the Φ_{E_k}-optimal values $v(k)$, $k = 1, 2, \ldots, m$, we can find the design that maximizes the minimal efficiency in the class $\mathbb{O}$, i.e., the design that is optimal with respect to the criterion

$$\Phi_{\mathbb{O}} : \mathcal{S}_+^m \to [0, \infty); \quad \Phi_{\mathbb{O}}(\mathbf{M}) = \min_{k=1,\ldots,m} \frac{\Phi_{E_k}(\mathbf{M})}{v(k)}. \tag{6}$$

The $\Phi_{\mathbb{O}}$-optimal design is the most efficiency stable design with respect to the class $\mathbb{O}$ and we will call it the $\mathbb{O}$-maximin efficient design, or, briefly, the maximin efficient design. Note that the maximin efficiency criterion is orthogonally invariant, i.e., $\Phi_{\mathbb{O}} \in \mathbb{O}$.

Since the functions Φ_{E_k} have in general complicated analytic properties, so does the function $\Phi_{\mathbb{O}}$. Therefore, to calculate the $\mathbb{O}$-maximin efficient design, the standard numerical procedures are difficult to apply. In this paper, we will show two possible approaches to solving this problem. In Section 2, we will make use of the form of the model (1) to calculate the $\mathbb{O}$-maximin efficient designs analytically. However, in general case, we have to resort to numerical procedures such as semidefinite programming, which will be used to compute the $\mathbb{O}$-maximin efficient designs in Section 3 for the model (2).

2. The model without a constant bias

Consider now the model (1). For $j \in \{0, \ldots, m\}$, let κ_j denote the uniform probability on the unit cube vertices from $\mathfrak{X}$ having j components equal to 1 and $m - j$ components equal to 0. We will call κ_j the j-vertex design. Let us extend the set of j-vertex designs to the set of neighbor-vertex designs κ_s, such that κ_s is a convex combination of $\kappa_{\lfloor s \rfloor}$ and $\kappa_{\lfloor s \rfloor + 1}$, specifically,

$$\kappa_s = \big(1 - (s - \lfloor s \rfloor)\big)\kappa_{\lfloor s \rfloor} + (s - \lfloor s \rfloor)\kappa_{\lfloor s \rfloor + 1} \qquad \text{for} \quad s \in [0, m].$$

As a trivial consequence of [11, Sec. 14.10, Claim I], we get the following proposition.

Proposition 1. *Let $\Phi \in \mathbb{O}$. Then there exists $s \in [0, m]$ such that the neighbor--vertex design κ_s is Φ-optimal for the model $(f, \mathfrak{X})$.*

Thus, we can restrict our search for optimal designs to the class of neighbor--vertex designs.

Theorem 1. *Let $m > 1$. The E_k-optimal values for the model* (1) *are $v(m) = m$, and if $1 \le k < m$, we have $v(k) = \frac{km}{4(m-1)}$ if m is even and $v(k) = \frac{k(m+1)}{4m}$ if m is odd.*

P r o o f. Using the results of [11, Sec. 14.10], it is easy to prove that for a neighbor vertex design κ_s, we have

$$\mathbf{M}(\kappa_s) = a_s^{(m)} \left(\mathbf{I}_m - \frac{1}{m} \mathbf{1}_m \mathbf{1}_m^T \right) + b_s^{(m)} \left(\frac{1}{m} \mathbf{1}_m \mathbf{1}_m^T \right),$$

where

$$a_s^{(m)} = \big(-2s\lfloor s \rfloor - s + \lfloor s \rfloor + \lfloor s \rfloor^2 + sm\big) / \big(m(m-1)\big)$$

and

$$b_s^{(m)} = \left(2s\lfloor s \rfloor + s - \lfloor s \rfloor - \lfloor s \rfloor^2\right)/m.$$

Hence, $\mathbf{M}(\kappa_s)$ is a completely symmetric matrix which implies that its vector of eigenvalues is

$$\lambda\big(\mathbf{M}(\kappa_s)\big) = \left(a_s^{(m)}, \dots, a_s^{(m)}, b_s^{(m)}\right)^T,$$

and, consequently, the E_k-optimal values follow directly after some simple algebra. □

Having derived the E_k-optimal values, we can now compute the $\mathbb{O}$-minimal efficiency of any given neighbor-vertex design κ_s.

Theorem 2. *Let $m > 1$, $s \in [0, m]$, and let κ_s be the neighbor-vertex design. Further, denote*

$$q(m, s) = -2s\lfloor s \rfloor - s + \lfloor s \rfloor + \lfloor s \rfloor^2 + sm.$$

Then

$$\operatorname{mineff}(\kappa_s|\mathbb{O}) = \begin{cases} \min\left\{\frac{4}{m^2} q(m,s), s/m\right\} & \text{if } m \text{ is even,} \\ \min\left\{\frac{4}{(m+1)(m-1)} q(m,s), s/m\right\} & \text{if } m \text{ is odd.} \end{cases} \tag{7}$$

P r o o f. From Theorem 1, it is clear that for a given m, the E_k-optimal values, $1 \le k < m$, grow linearly with k. Therefore, the E_k-efficiency of an arbitrary design ξ is at least as high as the E-efficiency of ξ. Therefore, the $\mathbb{O}$-minimal efficiency of ξ is simply the minimum of E_1- and E_m-efficiencies of ξ as follows from (5). Moreover,

$$\Phi_{E_m}(\kappa_s) = \operatorname{tr}\big(\mathbf{M}(\kappa_s)\big) = s,$$

that is, using Theorem 1, the E_m-efficiency of κ_s is s/m. □

Finally, we will show that, with the exception of the cases $m \equiv 2 (\text{mod } 4)$ and $m = 1$, the $\mathbb{O}$-maximin efficient design is the neighbor-vertex design $\kappa_{3m/4}$ and its $\mathbb{O}$-minimal efficiency is $3/4$.

Theorem 3. *Let $m \in \mathbb{N}$. Let*

$$s = \begin{cases} 1 & \text{if } m = 1, \\ \frac{3m}{4} & \text{if } m \not\equiv 2 (\text{mod } 4), \\ \frac{3m}{4} - \frac{1}{3m} & \text{if } m \equiv 2 (\text{mod } 4). \end{cases}$$

Then the neighbor vertex design κ_s is $\mathbb{O}$-maximin efficient for the model (1) *and*

$$\text{mineff}(\kappa_s|\mathbb{O}) = \begin{cases} 1 & \text{if } m = 1, \\ \frac{3}{4} & \text{if } m \not\equiv 2 (\text{mod } 4), \\ \frac{3}{4} - \frac{1}{3m^2} & \text{if } m \equiv 2 (\text{mod } 4). \end{cases}$$

Proof. If $m = 1$, the proof is trivial. Let $m > 1$. According to Theorem 2, we need to find $s \in [0, m]$ that maximizes $\text{mineff}(\kappa_s|\mathbb{O})$.

First, let m be even. In this case, we need to maximize the function $g(s) = \min\left\{\frac{4}{m^2} q(m, s), s/m\right\}$. Note that $4q(m, m/2)/m^2 = 1, 4q(m, m)/m^2 = 0$, and that the function $4q(m, \cdot)/m^2$ is decreasing on $[m/2, m]$. Now, as s/m is linear, we can restrict our search on the interval $s \in [m/2, m]$. Next, we know that the maximum of $g(s)$ is attained at the point which solves the equation $4q(m, s)/m^2 = s/m$. One can verify that the solution is $s = 3m/4$ if $m \equiv 0 (\text{mod } 4)$ and $s = 3m/4 - 1/(3m)$ if $m \equiv 2 (\text{mod } 4)$.

For odd m, the proof is analogous. □

Thus, the maximin efficient design κ_s requires that $100(1 - s + \lfloor s \rfloor)$ percent of weighings involve $\lfloor s \rfloor$ objects (and all possible combinations of $\lfloor s \rfloor$ objects appear the same number of times), and $100(s - \lfloor s \rfloor)$ percent of weighings involve $\lfloor s \rfloor + 1$ objects (and all possible combinations of $\lfloor s \rfloor + 1$ objects appear the same number of times). Of course, this is usually impossible with a finite number N of weighings; exceptions are, for instance: $m = 3$, $N \equiv 0 (\text{mod } 4)$; $m = 4$, $N \equiv 0 (\text{mod } 4)$; $m = 5$, $N \equiv 0 (\text{mod } 40)$; $m = 7$, $N \equiv 0 (\text{mod } 28)$, $m = 8$, $N \equiv 0 (\text{mod } 28)$ and $m = 9$, $N \equiv 0 (\text{mod } 336)$. However, the E_k-optimal values from Theorem 2 allow us to find a lower bound on the $\mathbb{O}$-minimal efficiency of any proposed design, which will be close to 3/4 if the proposed design itself is close to κ_s.

Note that, according to [8], the $\mathbb{O}$-minimal efficiency of the D-optimal design is $(m + 2)/\big(2(m + 1)\big)$ if m is even and $(m + 1)/(2m)$ if m is odd. For $m = 1, 2$, the D-optimal design coincides with the maximin efficient design. Nevertheless, for $m \to \infty$, the minimal efficiency of the D-optimal design converges to 1/2, which is substantially less than the limiting minimal efficiency 3/4 in the case of the maximin efficient design.

3. The model with a constant bias

In this section, we will consider the model (2) of spring balance weighing with a constant bias. Similarly to the previous section, we can restrict our search for optimal designs to convex combinations of j-vertex designs.

Proposition 2 (see [6]). *For any $\xi \in \Xi$ there exists a design $\overline{\kappa}$ that is a convex combination of the designs $\kappa_0, \dots, \kappa_d$, such that*

$$\Phi\big(\mathbf{M}(\overline{\kappa})\big) \geq \Phi\big(\mathbf{M}(\xi)\big) \qquad \textit{for all} \quad \Phi \in \mathbb{O}.$$

Therefore, for any orthogonally invariant criterion Φ, some convex combination of j-vertex designs is Φ-optimal.

For every vector $w = (w_0, \dots, w_d)^T$ of nonnegative weights summing to one, let $\bar{\kappa}_{w,d} = \sum_{k=1}^{d} w_j \kappa_j$. Then the information matrix of $\bar{\kappa}_{w,d}$ can be expressed as

$$\mathbf{M}(\bar{\kappa}_{w,d}) = \sum_{j=0}^{d} w_j \mathbf{M}(\kappa_j)$$

(see [6]), where

$$\mathbf{M}(\kappa_j) = \begin{pmatrix} \mathbf{H}_{j,d} & \frac{cj}{d}\,\mathbf{1}_d \\ \frac{cj}{d}\,\mathbf{1}_d^T & c^2 \end{pmatrix} \qquad \text{for all} \quad j = 0, 1, \dots, d$$

with

$$\mathbf{H}_{0,1} = 0, \quad \mathbf{H}_{1,1} = 1,$$

and

$$\mathbf{H}_{j,d} = \frac{j(d-j)}{d(d-1)}\,\mathbf{I}_d + \frac{j(j-1)}{d(d-1)}\,\mathbf{1}_d\mathbf{1}_d^T \qquad \text{for all} \quad d \geq 2, \; j = 0, 1, \dots, d.$$

In this case, the analytical computation of the maximin efficient designs would be very difficult. However, the form of the information matrix of an arbitrary admissible design $\bar{\kappa}_{w,d}$ makes it possible to use a numerical algorithm based on semidefinite programming. Semidefinite programming is a special subclass of convex mathematical programming and generalizes several standard optimization problems, such as linear or quadratic programming. In semidefinite programming, we optimize a linear function subject to linear constraints and linear matrix inequality constraints. The problems of finding E_k-optimal values and the maximin efficient designs were formulated as semidefinite programs in the paper [5].

First, we need to find the optimal values for the criteria of E_k-optimality. Using the methods developed in [5] and the SeDuMi toolbox for MATLAB [12], we have obtained the Φ_{E_k}-optimal values $v(k)$, $k = 1, \dots, d+1$, for selected values of d and c. Having these values, we were able to compute the maximin efficient designs (see Table 1).

TABLE 1. The weights for the designs κ_0, $\kappa_{\lfloor d/2 \rfloor}$, $\kappa_{\lfloor d/2 \rfloor+1}$ and κ_d forming the maximin efficient designs in the model (2) for $c = \frac{1}{4}, \frac{1}{2}, 1, 2, 4, 8$. The symbol eff denotes the corresponding minimal efficiency of the maximin design.

$c = \frac{1}{4}$	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.327	0.428	0	0.245	0.475
d=3	0.226	0.451	0	0.322	0.483
d=4	0.312	0.449	0	0.239	0.510
d=8	0.304	0.459	0	0.237	0.470

$c = \frac{1}{2}$	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.269	0.428	0	0.303	0.571
d=3	0.138	0.485	0	0.377	0.574
d=4	0.225	0.489	0	0.287	0.558
d=8	0.203	0.518	0	0.279	0.552

c=1	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.190	0.437	0	0.373	0.727
d=3	0.195	0.552	0	0.253	0.716
d=4	0.103	0.556	0	0.341	0.695
d=8	0.061	0.608	0	0.331	0.675

c=2	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.159	0.460	0	0.381	0.870
d=3	0.145	0	0.637	0.218	0.847
d=4	0.035	0.631	0	0.334	0.824
d=8	0.045	0	0.739	0.216	0.785

c=4	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.177	0.484	0	0.339	0.953
d=3	0.158	0	0.702	0.140	0.938
d=4	0.035	0.696	0	0.269	0.923
d=8	0.038	0	0.827	0.135	0.884

c=8	w_0	$w_{\lfloor d/2 \rfloor}$	$w_{\lfloor d/2 \rfloor+1}$	w_d	eff
d=2	0.205	0.495	0	0.300	0.986
d=3	0.192	0	0.735	0.073	0.980
d=4	0.063	0.732	0	0.205	0.974
d=8	0.066	0	0.892	0.041	0.955

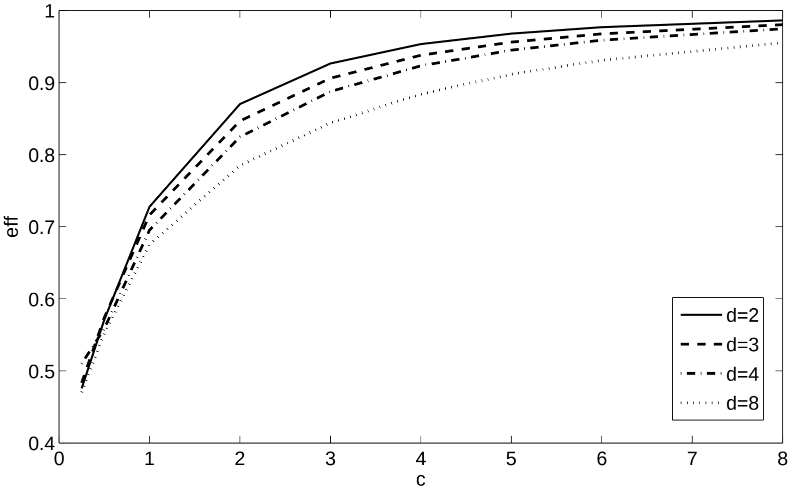

FIGURE 1. The $\mathbb{O}$-minimal efficiency (vertical axis) of maximin efficient designs for the model (2), plotted as a function of $c \in (0, 8]$ (horizontal axis), for $d = 2, 3, 4, 8$. The graphs were obtained by linear interpolation of values calculated for $c \in \{0.25, 0.5, 1, 2, 3, 4, 5, 6, 7, 8\}$.

We can see that with c converging to ∞ the $\mathbb{O}$-minimal efficiency of the maximin efficient design converges to 1 (cf. Table 1 or Figure 1). This is related to the fact that if in the model (2) we focus only on estimating the parameters of weights, then there exists a "universally" optimal design, cf. [3]. Note that Theorem 5 in [8] states that the efficiency of the D-optimal design with respect to any orthogonally invariant criterion is always at least $1/m$, where m is the number of parameters, which means that the minimal efficiency of the maximin efficient design must also be at least $1/m$. Hence, for $c \to 0$, the minimal efficiency of the maximin efficient design does not converge to 0. We calculated the maximin efficient design for $c = 0.1$, and the minimal efficiency of the maximin efficient design was about 0.43.

Note that, even in the case of a relatively large dimension, the minimal efficiency of the maximin efficient design does not significantly deteriorate. Further, note that, for $d \geq 3$, the maximin efficient design is not determined uniquely, and it turns out that for the cases we have analyzed, it is possible to choose its weights in such a way that only three of them are nonzero (see Table 1). Two of the nonzero weights are w_0 and w_d, and the third one either $w_{\lfloor d/2 \rfloor}$ or $w_{\lfloor d/2 \rfloor + 1}$.

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