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D-optimal minimax fractional factorial designs

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Abstract: The D-optimal minimax criterion is proposed to construct fractional factorial designs. The resulting designs are very efficient, and robust against misspecification of the effects in the linear model. The criterion was first proposed by Wilmut & Zhou (2011); their work is limited to two-level factorial designs, however. In this paper we extend this criterion to designs with factors having any levels (including mixed levels) and explore several important properties of this criterion. Theoretical results are obtained for construction of fractional factorial designs in general. This minimax criterion is not only scale invariant, but also invariant under level permutations. Moreover, it can be applied to any run size. This is an advantage over some other existing criteria. *The Canadian Journal of Statistics* 41: 325–340; 2013 © 2013 Statistical Society of Canada

Résumé: Les auteurs proposent le critère minimax D-optimal pour l'élaboration de plans factoriels fractionnaires. Les plans obtenus sont très efficaces et robustes à la spécification erronée des effets du modèle linéaire. Le critère a d'abord été proposé par Wilmut et Zhou (2011), dont les travaux se limitent aux plans factoriels à deux niveaux. Dans le présent article, les auteurs généralisent ce critère aux plans présentant des facteurs avec un nombre arbitraire de niveaux, y compris des niveaux mixtes, et ils examinent plusieurs propriétés importantes de ce critère. Ils obtiennent des résultats théoriques pour la construction de plans factoriels fractionnaires en général. Ce critère minimax est non seulement invariant à une transformation d'échelle, mais il est aussi invariant aux permutations de niveaux. De plus, il peut être appliqué à des essais de n'importe quelle taille. Il s'agit d'un avantage par rapport à d'autres critères existants. *La revue canadienne de statistique* 41: 325–340; 2013 © 2013 Société statistique du Canada

1. INTRODUCTION

Fractional factorial designs are very useful in industrial experiments. Various optimal design criteria have been studied based on the effect hierarchy principle (Mukerjee & Wu, 2006): namely (1) lower order effects are more important than higher order ones, and (2) the same-order effects are equally important. Box & Hunter (1961a, b) proposed the maximum resolution criterion. Since maximum resolution designs are not unique, the minimum aberration criterion was developed in Fries & Hunter (1980) to further discriminate among those designs to minimize the lower-order confounding. The clear effects criterion in Wu & Chen (1992) maximized the number of clear two-factor interactions. The maximum estimation capacity criterion in Sun (1993) aimed at selecting a design that could estimate all the main effects and as many two-factor interactions as possible. Other related developments can be found in Mukerjee & Wu (2006). Zhang et al. (2008) proposed a general minimum lower-order confounding criterion, which was based on a more detailed aliased effect-number pattern than the word length pattern.

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A D-optimal design minimizes the determinant of the covariance matrix of an estimator, and a minimum G_2-aberration design (Tang & Deng, 1999) minimizes the bias sequentially. Since it is important to consider both the variance and the bias of the estimator in a design criterion, Wilmut & Zhou (2011) studied a D-optimal minimax criterion to construct two-level fractional factorial designs. The criterion is based on the mean squared error of the least squares estimator (LSE). The resulting D-optimal minimax designs are very efficient and also robust against misspecification of the effects in the fitted model. Most design criteria for fractional factorial designs can only be applied to certain run sizes, especially for regular fractional factorial designs. However the D-optimal minimax criterion can be used for any run size.

The minimax criterion has been used to construct designs for many regression models. See, for example, Huber (1981), Wiens (1992), Fang & Wiens (2000), and Zhou (2001, 2008). The resulting designs are robust against small departures from model assumptions. Such departures include the misspecification of the response function (Huber, 1981; Wiens, 1992; Zhou, 2008), the misspecification of the correlation structure of the errors (Zhou, 2001), and the misspecification of the error variance (Fang & Wiens, 2000).

In this paper, we explore the D-optimal minimax criterion for fractional factorial designs and investigate several invariance properties. Theoretical results are derived to construct D-optimal minimax designs. Specific applications are given for three-level and mixed-level fractional factorial designs. The rest of this paper is organized as follows. Section 2 provides the basic terminologies and problem formulation. In Section 3, properties of D-optimal minimax designs are investigated and obtained. Examples of D-optimal minimax designs are presented in Section 4. Section 5 provides some concluding remarks. All proofs are given in the Appendix.

2. LINEAR MODEL AND D-OPTIMAL MINIMAX CRITERION

Suppose that there are k factors, $F_1, \ldots, F_k$, to be investigated through an experiment, where factor F_i has a_i ($a_i \geq 2$) levels, and a full factorial design has $N = a_1 a_2 \cdots a_k$ runs. Through a full factorial design, all the main effects and interactions can be estimated.

2.1. Orthogonal Effects

Let $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{(N-1)}$ be $N-1$ orthogonal columns containing all the main effects and interactions for a full factorial design with N runs. Define $l_i = (\mathbf{u}_i^\top \mathbf{u}_i)^{0.5}$ to be the vector norm of $\mathbf{u}_i$, $i = 1, \ldots, N-1$. For example, if $\mathbf{u}_i$ is the column representing the main effect for a two-level factor, then $\mathbf{u}_i$ has $N/2$ elements being -1 and $N/2$ elements being $+1$ and thus $l_i = N^{0.5}$. If $\mathbf{u}_i$ is the column representing the linear component of the main effect for a three-level factor, then $\mathbf{u}_i$ has $N/3$ elements being -1, $N/3$ elements being 0 and $N/3$ elements being $+1$ and thus $l_i = (2N/3)^{0.5}$. For the quadratic component of the main effect for a three-level factor, $\mathbf{u}_i$ has $N/3$ elements being -2, $2N/3$ elements being $+1$, and thus $l_i = (2N)^{0.5}$. Let the matrix $\mathbf{U} = (\mathbf{1}, \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{(N-1)})$, where $\mathbf{1}$ is the column of ones. It is obvious that $\mathbf{U}^\top\mathbf{U}$ is a diagonal matrix with elements $N, l_1^2, \ldots, l_{N-1}^2$, and we write $\mathbf{U}^\top\mathbf{U} = \mathrm{diag}\{N, l_1^2, \ldots, l_{N-1}^2\}$.

2.2. Linear Model

Let R_0 be a requirement set including all the main effects and some interaction effects. The main purpose of the experiment here is to efficiently estimate all the effects in R_0. Define a set of subscripts for the columns of $\mathbf{U}$ corresponding to the effects in R_0, that is, $J_0 = \{j : \mathbf{u}_j$ is a column representing an effect in $R_0\}$. Without loss of generality, we can assume $J_0 = \{1, 2, \ldots, m\}$, where m is the total number of effects in R_0 (say, by rearranging the columns in $\mathbf{U}$). Since the total number of main effect components is $\sum_{i=1}^{k}(a_i - 1)$ and the requirement set R_0 includes all the main effects, it is necessary that $m \geq \sum_{i=1}^{k}(a_i - 1)$.

Let y be the response variable for the experiment, and let x_j, $j \in J_0$, be the effects in R_0. The run size of the experiment is $n(\leq N)$. A linear model is assumed,

$$y_i = \theta_0 + \sum_{j=1}^{m} \theta_j x_{ij} + \epsilon_i, \quad i = 1, \ldots, n, \tag{1}$$

where x_{ij} is a design point of x_j, selected from column $\mathbf{u}_j$, and the errors ϵ_i's are i.i.d. random variables with mean 0 and variance σ^2. Let the matrix $\mathbf{U}_1 = (\mathbf{1}, \mathbf{u}_1, \ldots, \mathbf{u}_m)$ and $\mathbf{U}_2 = (\mathbf{u}_{m+1}, \ldots, \mathbf{u}_{(N-1)})$, then $\mathbf{U} = (\mathbf{U}_1, \mathbf{U}_2)$. Denote by $\mathbf{s}_i^\top$ the ith row of matrix $\mathbf{U}_1$, then the design space is $\mathbf{S} = \{\mathbf{s}_1, \ldots, \mathbf{s}_N\}$. An "optimal" fractional factorial design of n runs (points) will be selected from $\mathbf{S}$ without replacement such that it gives the "best" estimate for $\boldsymbol{\theta}_1 = (\theta_0, \theta_1, \ldots, \theta_m)^\top$ in (1).

2.3. Model Misspecification

If there are other significant effects that are mistakenly excluded in R_0, then the true response can be written as

$$E(y) = \theta_0 + \sum_{j=1}^{m} \theta_j x_j + f(x_1, \ldots, x_m), \tag{2}$$

where function f is called a departure function. To capture all possible departures from model (1), we define a class $\mathcal{F}$ of departure functions f as in Wilmut and Zhou (2011), where the function f satisfies two conditions:

(C1) The function f is orthogonal to regressors (effects) $x_0, x_1, \ldots, x_m$ on the design space $\mathbf{S}$, that is,

$$\sum_{i=1}^{N} f(u_{i1}, \ldots, u_{im}) u_{ij} = \sum_{i=1}^{N} f(\mathbf{s}_i) u_{ij} = 0, \quad j = 0, 1, \ldots, m, \tag{3}$$

where x_0 represents the term for θ_0, $u_{i0} = 1$, and u_{ij} is the ith element of column $\mathbf{u}_j$, $i = 1, \ldots, N$.

(C2) The function f is bounded on the design space $\mathbf{S}$, that is, for a given $\alpha \geq 0$,

$$\frac{1}{N} \sum_{i=1}^{N} f^2(u_{i1}, \ldots, u_{im}) = \frac{1}{N} \sum_{i=1}^{N} f^2(\mathbf{s}_i) \leq \alpha^2. \tag{4}$$

To find the functions in the class $\mathcal{F}$, define x_j to be the effect corresponding to column $\mathbf{u}_j$ in $\mathbf{U}$, $j = m+1, \ldots, N-1$. For $j \geq m+1$, x_j is an interaction, so it is a function of the main effects. Thus it is a function of effects $x_1, \ldots, x_m$. For $i = 1, \ldots, N$, let $\mathbf{z}_1(\mathbf{s}_i) = (u_{i1}, \ldots, u_{im})^\top$, $\mathbf{z}_2(\mathbf{s}_i) = (u_{i,m+1}, \ldots, u_{i,N-1})^\top$, and define two diagonal matrices:

$$\mathbf{V}_1 = \mathrm{diag}\{N, l_1^2, \ldots, l_m^2\}, \quad \mathbf{V}_2 = \mathrm{diag}\{l_{m+1}^2, \ldots, l_{N-1}^2\}. \tag{5}$$

The following lemma presents all the functions in $\mathcal{F}$.

Lemma 1. *Any function f in $\mathcal{F}$, satisfying conditions (C1) and (C2), has the following form:*

$$f(\mathbf{s}_i) = \mathbf{z}_2^\top(\mathbf{s}_i)\boldsymbol{\theta}_2, \quad i = 1, \ldots, N, \tag{6}$$

where $\boldsymbol{\theta}_2 \in R^{(N-m-1)}$ and $\frac{1}{N}\boldsymbol{\theta}_2^\top \mathbf{V}_2 \boldsymbol{\theta}_2 \leq \alpha^2$.

Lemma 1 shows that the departure function f in (2) is a linear combination of all the effects not in R_0. The magnitude of f is controlled by a bound in (C2), which puts a condition on the linear combination. The function f is involved in the bias of the LSE of $\boldsymbol{\theta}_1$ in (1), which will be discussed in the next subsection.

For two-level fractional factorial designs, it is clear that $l_i^2 = N$ for all $i = 1, \ldots, N-1$, so $\mathbf{V}_2 = N\mathbf{I}$, where $\mathbf{I}$ is the identity matrix. In this case, $\frac{1}{N}\boldsymbol{\theta}_2^\top \mathbf{V}_2 \boldsymbol{\theta}_2 \leq \alpha^2$ becomes $||\boldsymbol{\theta}_2|| \leq \alpha$, and the result in Lemma 1 reduces to that of Wilmut & Zhou (2011, Lemma 1).

2.4. D-Optimal Minimax Criterion

Model (1) can be written in matrix form as

$$\mathbf{y} = \mathbf{Z}_1\boldsymbol{\theta}_1 + \boldsymbol{\epsilon}, \tag{7}$$

where $\mathbf{y} = (y_1, \ldots, y_n)^\top$, $\mathbf{Z}_1$ is the $n \times (m+1)$ model matrix for the requirement set $\mathcal{R}_0$ and each row of $\mathbf{Z}_1$ is a selected row of $\mathbf{U}_1$ or a point in $\mathbf{S}$, and $\boldsymbol{\epsilon}$ is the error vector having mean $\mathbf{0}$ and variance matrix $\sigma^2\mathbf{I}_n$. However the possible true model is (2). From Lemma 1, the true model can be written as

$$\mathbf{y} = \mathbf{Z}_1\boldsymbol{\theta}_1 + \mathbf{Z}_2\boldsymbol{\theta}_2 + \boldsymbol{\epsilon}, \tag{8}$$

where $\mathbf{Z}_2$ is the $n \times (N - m - 1)$ model matrix for the effects not in $\mathcal{R}_0$, and each row of $\mathbf{Z}_2$ is a selected row of $\mathbf{U}_2$.

From model (7), the LSE of $\boldsymbol{\theta}_1$ is given by

$$\hat{\boldsymbol{\theta}}_1 = (\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{y}.$$

The variance and bias of the LSE are, respectively,

$$\begin{aligned}\mathrm{Cov}(\hat{\boldsymbol{\theta}}_1) &= \sigma^2(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1},\\ \mathrm{Bias}(\hat{\boldsymbol{\theta}}_1) &= E(\hat{\boldsymbol{\theta}}_1) - \boldsymbol{\theta}_1 = (\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\boldsymbol{\theta}_2\end{aligned}$$

and the mean squared error is

$$\begin{aligned}\mathrm{MSE}(\hat{\boldsymbol{\theta}}_1, \mathbf{Z}_1, \boldsymbol{\theta}_2) &= \mathrm{Cov}(\hat{\boldsymbol{\theta}}_1) + \mathrm{Bias}(\hat{\boldsymbol{\theta}}_1)\mathrm{Bias}^\top(\hat{\boldsymbol{\theta}}_1)\\ &= \sigma^2(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1} + (\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\boldsymbol{\theta}_2\boldsymbol{\theta}_2^\top\mathbf{Z}_2^\top\mathbf{Z}_1(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}.\end{aligned} \tag{9}$$

For a fixed run size n, the D-optimal minimax criterion for constructing fractional factorial designs for model (7) is to find a design $\mathbf{Z}_1^*$ minimizing the following loss function

$$\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) = \max_{\boldsymbol{\theta}_2} \det\left(\mathrm{MSE}(\hat{\boldsymbol{\theta}}_1, \mathbf{Z}_1, \boldsymbol{\theta}_2)\right), \tag{10}$$

where $\boldsymbol{\theta}_2$ satisfies $\frac{1}{N}\boldsymbol{\theta}_2^\top\mathbf{V}_2\boldsymbol{\theta}_2 \leq \alpha^2$. The design $\mathbf{Z}_1^*$ is called a D-optimal minimax design for model (7). The minimax problem is difficult in general, but here we are able to find an explicit expression for $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$. The result for $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ allows us to investigate various properties of D-optimal minimax designs.

Theorem 1. *The loss function in (10) equals to*

$$\mathcal{L}_{\rm D}(\mathbf{Z}_1) = \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top \mathbf{Z}_1 \mathbf{V}_1^{-1/2}))}{\det(\mathbf{Z}_1^\top \mathbf{Z}_1)}, \tag{11}$$

where $\lambda_{\min}(\,)$ denotes the smallest eigenvalue of a matrix, and matrix $\mathbf{V}_1$ is given in (5).

A D-optimal minimax design minimizes $\mathcal{L}_{\rm D}(\mathbf{Z}_1)$. An explicit form for $\mathcal{L}_{\rm D}(\mathbf{Z}_1)$ is obtained in Theorem 1, thus the minimax problem associated with the D-optimal minimax criterion becomes a minimization problem. D-optimal minimax designs are still hard to derive analytically but can be found numerically. However, many theoretical properties have been obtained, as presented in the next section.

For two-level fractional factorial designs, since $l_i^2 = N$ for all $i = 1, \ldots, N-1$, we have $\mathbf{V}_1 = N\mathbf{I}$. In this case, $1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top \mathbf{Z}_1 \mathbf{V}_1^{-1/2}) = 1 - \frac{1}{N}\lambda_{\min}(\mathbf{Z}_1^\top \mathbf{Z}_1)$, and the result in Theorem 1 becomes the result in Wilmut & Zhou (2011, Theorem 1).

3. PROPERTIES OF D-OPTIMAL MINIMAX DESIGNS

For a given requirement set R_0, a D-optimal minimax design of n runs can be selected from the N rows of matrix $\mathbf{U}_1$. If the columns of $\mathbf{U}_1$ or $\mathbf{U}$ are rescaled with different vector norms, is the D-optimal minimax design scale invariant? Scale invariance is a property that often fails for A- and E-optimality, even in the absence of robustness consideration. But it holds for D-optimality without robustness. Also factor levels can be coded differently, and in particular the levels can be permuted. Is the D-optimal minimax design permutation invariant? Two results are derived in this section to provide positive answers to these questions. In addition, a result about the loss function and the relationship between D-optimal designs and D-optimal minimax designs are investigated.

3.1. Scale Invariance

Suppose the columns of $\mathbf{U}$ are multiplied, respectively, by positive constants $b_1, \ldots, b_{N-1}$, namely $\tilde{\mathbf{u}}_j = \mathbf{u}_j b_j$, $j = 1, \ldots, N-1$. Define two diagonal matrices $\mathbf{B}_1 = \text{diag}\{1, b_1, \ldots, b_m\}$ and $\mathbf{B}_2 = \text{diag}\{b_{m+1}, \ldots, b_{N-1}\}$, and let $\mathbf{B} = \mathbf{B}_1 \oplus \mathbf{B}_2$ and $\tilde{\mathbf{U}} = \mathbf{U}\mathbf{B}$. The vector norms of the columns in $\tilde{\mathbf{U}}$ become $\tilde{l}_j = \|\tilde{\mathbf{u}}_j\| = l_j b_j$, $j = 1, \ldots, N-1$. Let $\tilde{\mathbf{V}}_1 = \text{diag}\{N, \tilde{l}_1^2, \ldots, \tilde{l}_m^2\}$. It is obvious that

$$\tilde{\mathbf{V}}_1 = \mathbf{B}_1 \mathbf{V}_1 \mathbf{B}_1. \tag{12}$$

Using the rescaled effects, we fit the following linear model,

$$\mathbf{y} = \tilde{\mathbf{Z}}_1 \boldsymbol{\theta}_1 + \boldsymbol{\epsilon}, \tag{13}$$

where $\tilde{\mathbf{Z}}_1 = \mathbf{Z}_1 \mathbf{B}_1$ and $\mathbf{Z}_1$ is the same as in model (7).

Theorem 2. *Suppose $\mathbf{Z}_1^*$ is a D-optimal minimax design for (7). Then a D-optimal minimax design for (13) is $\tilde{\mathbf{Z}}_1^* = \mathbf{Z}_1^* \mathbf{B}_1$, which implies that the same n rows are selected in the two D-optimal minimax designs for (7) and (13).*

Theorem 2 shows that a D-optimal minimax design is scale invariant. This implies that a D-optimal minimax design for a model can be called a D-optimal minimax design for a requirement set R_0.

3.2. Permutation Invariance

A factor level permutation may be applied to more than one factor, and each factor can be permuted differently. Assume that columns $\bar{\mathbf{u}}_j$'s are the result of a permutation. Define a class of permutations $\Pi = \{\pi : \ \bar{\mathbf{u}}_j = \pm\mathbf{u}_j \text{ for all } j = 1, \ldots, N-1\}$. In fact, if $\bar{\mathbf{u}}_j = \pm\mathbf{u}_j$ for all the main effects, then it is true for all the interactions. Write $\bar{\mathbf{u}}_j = q_j\mathbf{u}_j$ with $q_j = \pm 1$, and define a diagonal matrix $\mathbf{Q}_1 = \mathrm{diag}\{1, q_1, \ldots, q_m\}$. Let $\bar{\mathbf{Z}}_1 = \mathbf{Z}_1\mathbf{Q}_1$, and a fitted model under a level permutation in Π is

$$\mathbf{y} = \bar{\mathbf{Z}}_1\boldsymbol{\theta}_1 + \boldsymbol{\epsilon}. \tag{14}$$

Theorem 3 below shows that D-optimal minimax designs are invariant under permutations in Π.

Theorem 3. *The loss functions for models (7) and (14) are identical, that is,* $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) = \mathcal{L}_{\mathrm{D}}(\bar{\mathbf{Z}}_1)$.

Theorem 3 can also be interpreted as that D-optimal minimax designs may not be unique for a requirement set R_0. Suppose $\mathbf{Z}_1^*$ is a D-optimal minimax design. If there exists a diagonal matrix $\mathbf{Q}_1$ with elements ± 1 such that $\mathbf{Z}_1^*\mathbf{Q}_1$ is a possible design on design space $\mathbf{S}$, then $\mathbf{Z}_1^*\mathbf{Q}_1$ is also a D-optimal minimax design. For example, for a two-level factor, it can be done by switching the two levels; for a three-level factor, it can be done by keeping the middle level the same and switching the other two levels.

3.3. More Theoretical Properties

Theorem 4. *The loss function* $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^*)$ *is a decreasing function of run size n, where* $\mathbf{Z}_1^*$ *is a D-optimal minimax design for (7). For* $n = N$, *we have* $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^*) = \sigma^{2(m+1)}/(N\prod_{i=1}^m l_i^2)$.

Theorem 4 establishes some lower bounds for the loss function $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^*)$, which will be illustrated in Examples 2 and 3 in the next section. A better lower bound (not proved yet) is proposed and discussed in Section 5.

Now let us examine the relationship between D-optimal designs and D-optimal minimax designs. Define $v = N\alpha^2/\sigma^2$, $\phi_1(\mathbf{Z}_1) = \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2})$ and $\phi_2(\mathbf{Z}_1) = \det(\mathbf{Z}_1^\top\mathbf{Z}_1)$, then $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) = \sigma^{2(m+1)}[1 + v(1-\phi_1(\mathbf{Z}_1))]/\phi_2(\mathbf{Z}_1)$. A D-optimal design maximizes $\phi_2(\mathbf{Z}_1)$. If $v = 0$, minimizing $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ is equivalent to maximizing $\phi_2(\mathbf{Z}_1)$, then a D-optimal minimax design is a D-optimal design. For $0 < v < \infty$, D-optimal minimax designs may not be the same as D-optimal designs. However, if a design maximizes both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$, then it is a D-optimal minimax design and does not depend on v. For $v \to \infty$, minimizing $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ is equivalent to maximizing $\phi_1(\mathbf{Z}_1)$. From Theorem 2, D-optimal minimax designs are scale invariant, so we can scale the columns of $\mathbf{U}$ and make their norms to be the same, say $l_i = N^{0.5}$. Then maximizing $\phi_1(\mathbf{Z}_1)$ is equivalent to maximizing $\lambda_{\min}(\mathbf{Z}_1^\top\mathbf{Z}_1)$, which is the E-optimal design criterion. Often D-optimal minimax designs maximize both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$, so they are both D-optimal and E-optimal designs.

TABLE 1: D-optimal minimax design in Example 1.

Factor/run	1	2	3	4	5	6	7	8	9
F_1	0	1	2	0	1	2	0	1	2
F_2	0	0	0	1	1	1	2	2	2
F_3	0	2	1	1	0	2	2	1	0

4. EXAMPLES

In this section, we present three examples of D-optimal minimax designs including one for mixed-level and two for three-level fractional factorial designs. In Example 1, we show that D-optimal minimax designs do not depend on the value of v, and many D-optimal minimax designs can be generated using the result in Theorem 3. In Example 2, we confirm the result in Theorem 4 and also examine the relationship between D-optimal designs and D-optimal minimax designs. All the D-optimal minimax designs in Examples 1 and 2 are D-optimal designs, so they are highly efficient. The results in Examples 1 and 2 are obtained using a complete search method. Example 3 provides the detail to apply a simulated annealing algorithm to find D-optimal minimax designs.

Example 1. Suppose we want to construct a D-optimal minimax design with $n = 9$ runs and three three-level factors F_1, F_2 and F_3. Consider a requirement set $R_0 = \{x_{1L}, x_{1Q}, x_{2L}, x_{2Q}, x_{3L}, x_{3Q}\}$, where x_{iL} and x_{iQ} are the linear and quadratic components of the main effect of factor F_i, $i = 1, 2, 3$. The three levels (0, 1, 2) of F_i are coded as $(-1, 0, +1)$ in x_{iL} and $(+1, -2, +1)$ in x_{iQ}. A full factorial design has $N = 3^3 = 27$ runs. Since $27!/(9!\ 18!) = 4{,}686{,}825$, a complete search is possible to find a D-optimal minimax design. In the loss function $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$, we set $v = 1$ to search for D-optimal minimax designs first. By minimizing $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$, D-optimal minimax designs were obtained. Table 1 presents one of them. All the D-optimal minimax designs give $\phi_1(\mathbf{Z}_1) = 1/3$ and $\phi_2(\mathbf{Z}_1) = 11, 337, 408$, and both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$ are maximized. Thus D-optimal minimax designs do not depend on the value of v in this

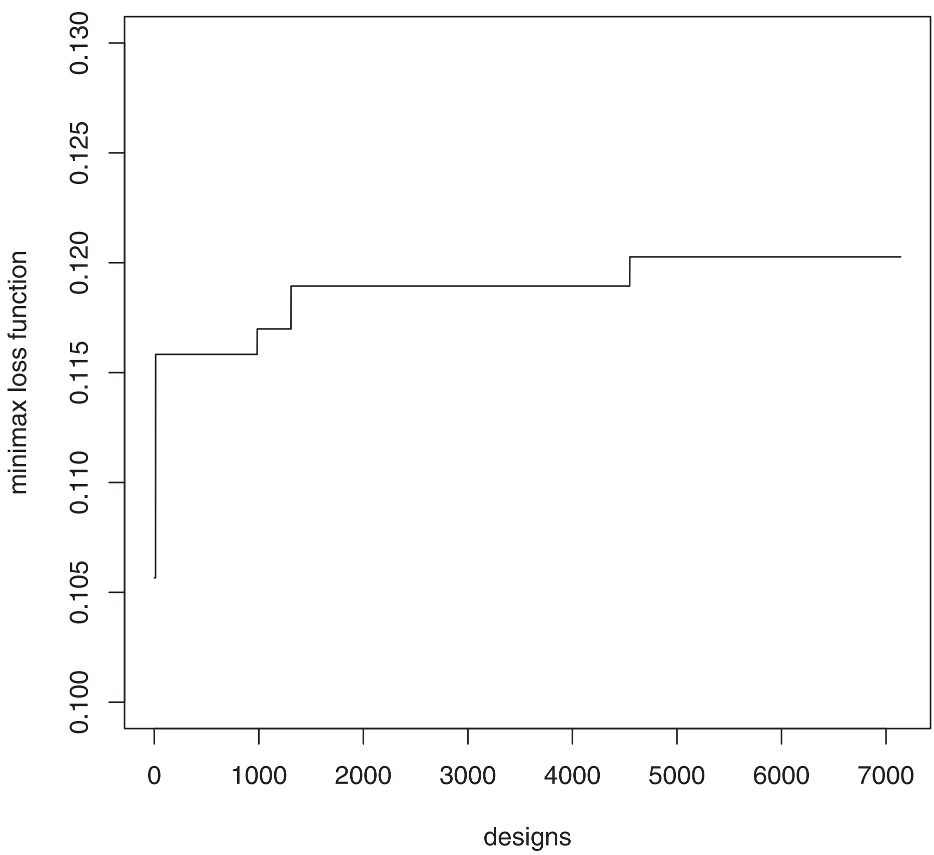

FIGURE 1: Loss function $(\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1))^{1/(m+1)}$ for the first 5 classes in Example 1.

example, and they are also D-optimal designs for R_0. Notice that the design in Table 1 is a regular fractional factorial design with the defining relation: $F_3 = F_1^2 F_2$. Applying the result in Theorem 3, we can get a few D-optimal minimax designs from Table 1 by permuting levels 0 and 2 within each factor, since the quadratic component remains unchanged and the linear component changes a sign. We can permute the levels for any number of factors.

Using the loss function $\mathcal{L}_D(\mathbf{Z}_1)$, those 4,686,825 designs can be grouped into several equivalence classes, but the number of classes is usually quite large. There are more than 40 classes in this example, and a plot of the smallest values of the loss function with $v = 1$ for the first 5 classes versus the designs is given in Figure 1. There are 12 D-optimal minimax designs (the first class), 972 in the second class, 324 in the third class, 3,240 in the fourth class, and 2,592 in the fifth class. □

Example 2. Consider an experiment with three factors: Factors F_1 and F_2 with three levels, while F_3 with two levels. Suppose we want to estimate all the main effects, interaction between F_1 and F_3, and interaction between F_2 and F_3. The requirement set is then $R_0 = \{x_{1L}, x_{1Q}, x_{2L}, x_{2Q}, x_3, x_{1L}x_3, x_{1Q}x_3, x_{2L}x_3, x_{2Q}x_3\}$, where x_{iL} and x_{iQ} are the linear and quadratic components of the main effect of factor F_i, $i = 1, 2$, and x_3 is the main effect of F_3. The

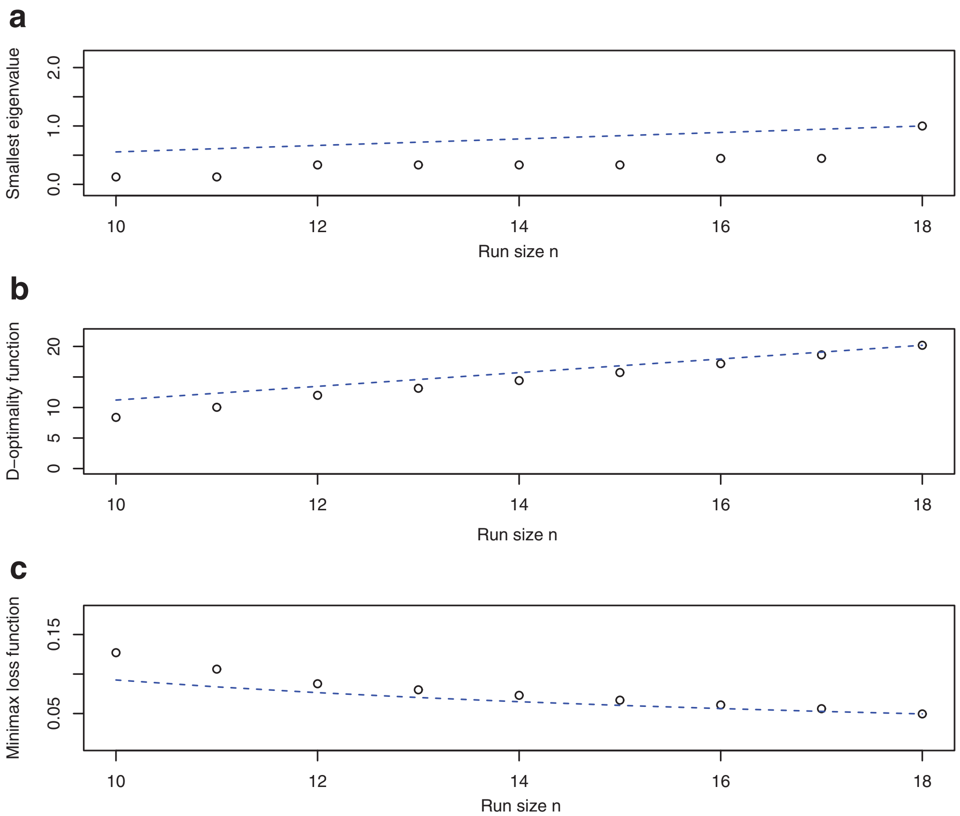

FIGURE 2: Functions in Example 2: (a) $\max \phi_1(\mathbf{Z}_1)$ versus n, (b) $(\max \phi_2(\mathbf{Z}_1))^{1/(m+1)}$ versus n, (c) $(\min \mathcal{L}_D(\mathbf{Z}_1))^{1/(m+1)}$ versus n, with $v = 1$ and $\sigma^2 = 1$. The circles represent the actual function values, while the dotted lines are upper bounds in (a) and (b) and a lower bound in (c).

TABLE 2: Two designs for $n = 10$ in Example 2.

	Run	1	2	3	4	5	6	7	8	9	10
Design d_1											
F_1		0	1	2	0	0	1	2	2	0	1
F_2		0	0	0	1	2	0	0	1	2	2
F_3		−1	−1	−1	−1	−1	+1	+1	+1	+1	+1
Function	$\phi_1 = 0.08390$			$\phi_2 = 1{,}719{,}926{,}784$				$\mathcal{L}_{\mathrm{D}}^{1/(m+1)} = 0.12726$			
Design d_2											
F_1		0	1	2	0	2	0	1	2	1	2
F_2		0	0	0	1	2	0	0	0	1	2
F_3		−1	−1	−1	−1	−1	+1	+1	+1	+1	+1
Function	$\phi_1 = 0.12732$			$\phi_2 = 1{,}719{,}926{,}784$				$\mathcal{L}_{\mathrm{D}}^{1/(m+1)} = 0.12697$			

three levels (0, 1, 2) of F_i ($i = 1$ and 2) are coded as $(-1, 0, +1)$ in x_{iL} and $(+1, -2, +1)$ in x_{iQ}, and the two levels of F_3 are coded as -1 and $+1$. A full factorial design has $N = 2 \times 3^2 = 18$ runs. We construct D-optimal minimax designs for various run sizes, $n = 10, 11, \ldots, 18$, using a complete search. Figure 2 presents three plots: (a) $\max \phi_1(\mathbf{Z}_1)$ versus n, (b) $(\max \phi_2(\mathbf{Z}_1))^{1/(m+1)}$ versus n, and (c) $(\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1))^{1/(m+1)}$ (with $v = 1$ and $\sigma^2 = 1$) versus n. It shows that $\max \phi_1(\mathbf{Z}_1)$ and $\max \phi_2(\mathbf{Z}_1)$ are increasing functions of n, and $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ is a monotonic decreasing function of n. This is consistent with Theorem 4. From the numerical results, we also notice that some D-optimal designs are not D-optimal minimax designs and some designs maximizing $\phi_1(\mathbf{Z}_1)$ are not D-optimal minimax designs either. The D-optimal minimax designs maximize both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$, so they do not depend on v. Table 2 presents two designs d_1 and d_2 for $n = 10$, where d_1 is a D-optimal design but not a D-optimal minimax design, while d_2 maximizes both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$ and thus is a D-optimal minimax design. Table 3 gives two designs d_3 and d_4

TABLE 3: Two designs for $n = 15$ in Example 2.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Design d_3															
F_1	0	1	2	0	1	2	0	1	2	0	1	0	2	1	2
F_2	0	0	0	1	1	1	2	2	2	0	0	1	1	2	2
F_3	−1	−1	−1	−1	−1	−1	−1	−1	−1	+1	+1	+1	+1	+1	+1
Function	$\phi_1 = 0.33333$				$\phi_2 = 835{,}884{,}417{,}024$					$\mathcal{L}_{\mathrm{D}}^{1/(m+1)} = 0.06760$					
Design d_4															
F_1	0	1	2	0	1	2	0	1	0	1	2	1	2	0	1
F_2	0	0	0	1	1	1	2	2	0	0	0	1	1	2	2
F_3	−1	−1	−1	−1	−1	−1	−1	−1	+1	+1	+1	+1	+1	+1	+1
Function	$\phi_1 = 0.33333$				$\phi_2 = 928{,}760{,}463{,}360$					$\mathcal{L}_{\mathrm{D}}^{1/(m+1)} = 0.06689$					

TABLE 4: D-optimal minimax design for $n = 27$ in Example 3.

Run	F_1	F_2	F_3	F_4	Run	F_1	F_2	F_3	F_4
1	1	0	0	0	15	1	2	1	1
2	2	0	0	0	16	2	0	2	1
3	2	2	0	0	17	2	1	2	1
4	0	0	1	0	18	2	2	2	1
5	0	1	1	0	19	1	1	0	2
6	2	1	1	0	20	2	1	0	2
7	1	1	2	0	21	1	2	0	2
8	0	2	2	0	22	2	0	1	2
9	1	2	2	0	23	0	2	1	2
10	0	0	0	1	24	2	2	1	2
11	0	1	0	1	25	0	0	2	2
12	0	2	0	1	26	1	0	2	2
13	1	0	1	1	27	0	1	2	2
14	1	1	1	1					

for $n = 15$, where d_3 maximizes $\phi_1(\mathbf{Z}_1)$, but it is not a D-optimal minimax design or D-optimal design. Design d_4 maximizes both $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$ and is a D-optimal minimax design. □

If N is large, $N!/(n!(N-n)!)$ can be very large and it is not feasible to do a complete search to find D-optimal minimax designs. In this case, a simulated annealing algorithm can be used to search for D-optimal minimax designs. This algorithm has been implemented to find optimal/robust designs in the literature, and it is shown to be very effective. See, for example, Fang & Wiens (2000) and Wilmut & Zhou (2011). Since the denominator of $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$, $\phi_2(\mathbf{Z}_1)$, can be zero for some designs and it will cause problems in the computation, we minimize the function $-1/\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) = -\phi_2(\mathbf{Z}_1)/(1 + v(1 - \phi_1(\mathbf{Z}_1)))$ instead of $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$. A typical example is illustrated below.

Example 3. Suppose there are four factors, F_1, F_2, F_3, and F_4, and each has three levels. A requirement set includes all the main effects and interaction effects between F_1 and F_2, that is, $R_0 = \{x_{1L}, x_{1Q}, x_{2L}, x_{2Q}, x_{3L}, x_{3Q}, x_{4L}, x_{4Q}, x_{1L}x_{2L}, x_{1L}x_{2Q}, x_{1Q}x_{2L}, x_{1Q}x_{2Q}\}$ with $m = 12$ effects. These effects are coded the same as in Example 1. A full factorial design has $N = 81$ runs. We use the annealing algorithm in Wilmut & Zhou (2011) to construct D-optimal minimax designs for $n = 27$ and 30. In the algorithm, several parameters are set as follows: the initial temperature $T_0 = 20$, the number of designs searched at each temperature $N_T = 2{,}000$, and the number of temperature changes $M_0 = 100$. Often it is hard to determine if a numerical result gives a global optimization solution. The following procedure is further implemented.

(1) Run the algorithm several times with different initial designs and pick the best numerical result with the minimum loss function $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$.
(2) Plot the loss function versus the number of iterations to see if the function converges.

TABLE 5: D-optimal minimax design for $n = 30$ in Example 3.

Run	F_1	F_2	F_3	F_4	Run	F_1	F_2	F_3	F_4
1	0	0	0	0	16	0	2	1	1
2	2	0	0	0	17	1	2	1	1
3	0	2	0	0	18	2	0	2	1
4	1	2	0	0	19	2	1	2	1
5	1	0	1	0	20	1	2	2	1
6	1	1	1	0	21	2	0	0	2
7	2	1	1	0	22	2	1	0	2
8	0	1	2	0	23	0	2	0	2
9	0	2	2	0	24	1	2	0	2
10	2	2	2	0	25	2	0	1	2
11	1	0	0	1	26	0	1	1	2
12	0	1	0	1	27	2	2	1	2
13	1	1	0	1	28	0	0	2	2
14	2	2	0	1	29	1	0	2	2
15	0	0	1	1	30	1	1	2	2

In this example, we run the algorithms 10 times. For $n = 27$, the resulting D-optimal minimax design obtained from the algorithm is presented in Table 4. This design gives $\mathbf{Z}_1^\top \mathbf{Z}_1 = \frac{1}{3}\mathbf{U}_1^\top \mathbf{U}_1 = \mathrm{diag}\{27, 18, 54, 18, 54, 18, 54, 18, 54, 12, 36, 36, 108\}$ and $\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top \mathbf{Z}_1 \mathbf{V}_1^{-1/2} = \frac{1}{3}\mathbf{I}$. For $n = 30$, the resulting D-optimal minimax design obtained from the algorithm is given in Table 5, and the design gives $\phi_1(\mathbf{Z}_1) = 1/3$, $(\phi_2(\mathbf{Z}_1))^{(1/13)} = 35.2841$, and $(\mathcal{L}_\mathrm{D}(\mathbf{Z}_1))^{(1/13)} = 0.0295$. The loss function converges, as shown in Figure 3 for the plots of $\phi_1(\mathbf{Z}_1)$, $(\phi_2(\mathbf{Z}_1))^{(1/13)}$ and $(\mathcal{L}_\mathrm{D}(\mathbf{Z}_1))^{(1/13)}$ versus the accepted designs in the annealing algorithm (for the case $n = 30$). □

5. CONCLUSION

D-optimal minimax criterion is studied for constructing fractional factorial designs. This criterion is scale invariant and also level permutation invariant within some classes of permutations. General theoretical results are derived for factors with various levels. The pioneering study of Wilmut & Zhou (2011) can be viewed as a special case of our results.

D-optimal minimax designs are nearly as efficient as D-optimal designs, and they are also robust against the misspecification of the effects in the requirement set. D-optimal designs may not be D-optimal minimax designs, but D-optimal minimax designs are often both D-optimal designs and E-optimal designs. In addition, D-optimal minimax criterion can be applied to any run size, while most criteria for fractional factorial designs are limited to run size.

For two-level fractional factorial designs, we have $\mathbf{U}_1^\top \mathbf{U}_1 = N\,\mathbf{I}$ and $\mathbf{V}_1 = N\,\mathbf{I}$. If a design gives $\mathbf{Z}_1^\top \mathbf{Z}_1 = \frac{n}{N}\mathbf{U}_1^\top \mathbf{U}_1$, then $\mathbf{Z}_1^\top \mathbf{Z}_1 = n\,\mathbf{I}$ and $\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top \mathbf{Z}_1 \mathbf{V}_1^{-1/2} = \frac{n}{N}\mathbf{I}$. Therefore $\phi_1(\mathbf{Z}_1) = n/N$ and $\phi_2(\mathbf{Z}_1) = n^{(m+1)}$ are both maximized, and the design is a D-optimal minimax design. This result is shown in Wilmut & Zhou (2011) to get upper bounds for $\phi_1(\mathbf{Z}_1)$ and $\phi_2(\mathbf{Z}_1)$ and a lower bound for $\mathcal{L}_\mathrm{D}(\mathbf{Z}_1)$. For some values of n and some requirement sets, these upper and lower

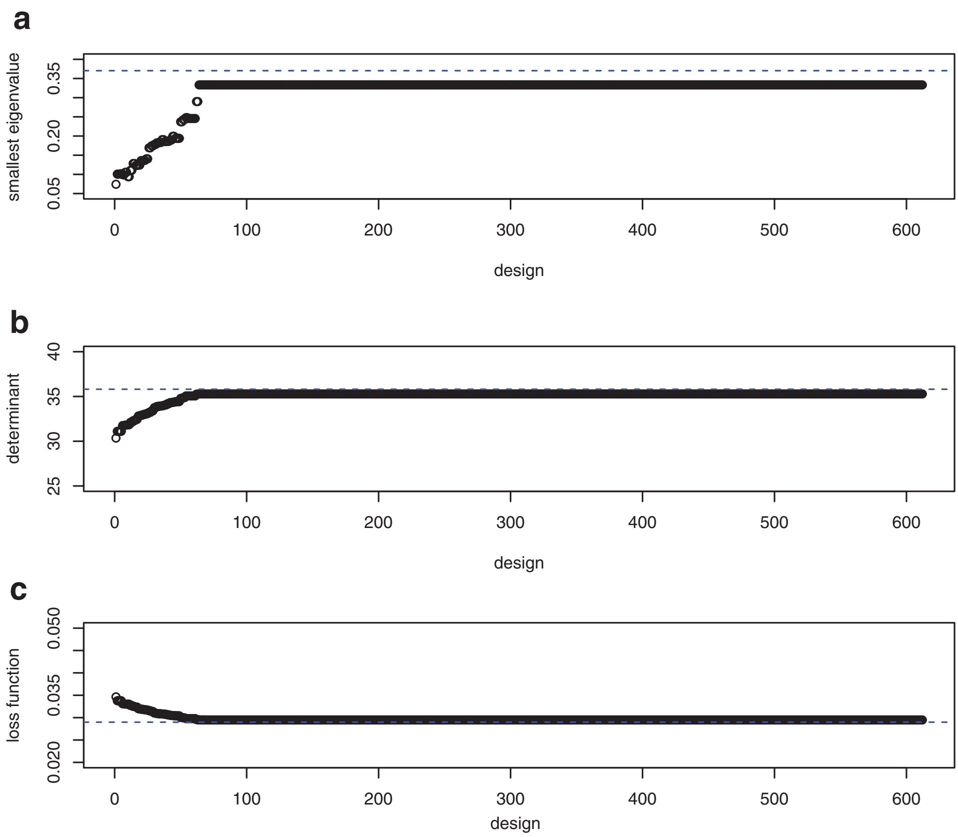

FIGURE 3: Functions in Example 3 (for $n = 30$): (a) $\phi_1(\mathbf{Z}_1)$ versus the accepted designs in the annealing algorithm, (b) $(\phi_2(\mathbf{Z}_1))^{1/(m+1)}$ versus the accepted designs, (c) $(\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1))^{1/(m+1)}$ versus the accepted designs, with $v = 1$ and $\sigma^2 = 1$. The horizontal dotted lines are corresponding upper and lower bounds according to $\mathbf{Z}_1^\top \mathbf{Z}_1 = \frac{n}{N}\mathbf{U}_1^\top \mathbf{U}_1$.

bounds can be reached. This implies that if a regular fractional factorial design exists for a given run size n and the design allows us to estimate all the effects in the requirement set, then the design is a D-optimal design and a D-optimal minimax design.

However, it is hard to prove the above result for three-level or mixed-level designs and it remains an open problem. Specifically, for three-level or mixed-level fractional factorial designs, it is conjectured that

$$\phi_1(\mathbf{Z}_1) \le \phi_1(\mathbf{Z}_1^o), \quad \phi_2(\mathbf{Z}_1) \le \phi_2(\mathbf{Z}_1^o), \quad \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) \ge \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^o), \tag{15}$$

if $\mathbf{Z}_1^o$ satisfies that $\mathbf{Z}_1^{o\top}\mathbf{Z}_1^o = \frac{n}{N}\mathbf{U}_1^\top \mathbf{U}_1$. Notice that for some values of n, there may not exist such a design $\mathbf{Z}_1^o$. In Figures 2 and 3, the dotted lines are the corresponding functions computed from $\phi_1(\mathbf{Z}_1^o)$, $\phi_2(\mathbf{Z}_1^o)$ and $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^o)$. It is clear that these lines provide good upper and lower bounds for the loss functions in Examples 2 and 3. In Example 1, the lower bound is very close to $\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ as indicated in Figure 4. It is also interesting to notice that when $n = 9$, 18, and 27, $(\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1))^{1/(m+1)}$ is the same as the lower bound. This indicates that there exists a design $\mathbf{Z}_1^o$

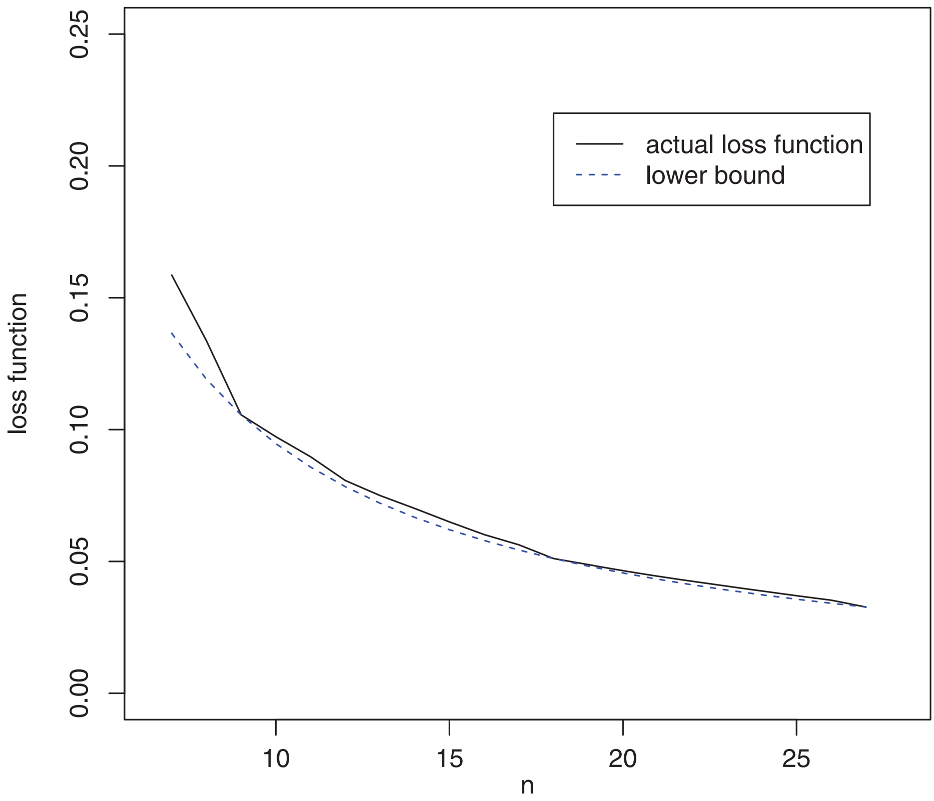

FIGURE 4: The loss function $(\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1))^{1/(m+1)}$ and its lower bound versus run size n in Example 1.

satisfying $\mathbf{Z}_1^{o\top}\mathbf{Z}_1^o = \frac{n}{N}\mathbf{U}_1^\top\mathbf{U}_1$ for $n = 9$, 18 and 27. Similar to Figure 1 in Bingham & Chipman (2007), the plot of $\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ versus n can be very useful to select the run size n. In the case where it is not feasible to compute the $\min \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$, the lower bound of $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$ versus n can be plotted.

APPENDIX

Proof of Lemma 1. Define vector $\mathbf{f}_N = (f(\mathbf{s}_1), \ldots, f(\mathbf{s}_N))^\top$, then condition (C1) can be written as $\mathbf{U}_1^\top\mathbf{f}_N = \mathbf{0}$. Since the columns of $\mathbf{U}$ are orthogonal, we have $\mathbf{U}_1^\top\mathbf{U}_2 = \mathbf{0}$. Notice that the ranks of $\mathbf{U}_1$ and $\mathbf{U}_2$ are $m+1$ and $N-m-1$ respectively. From linear algebra, it is obvious that $\mathbf{f}_N = \mathbf{U}_2\boldsymbol{\theta}_2$ with $\boldsymbol{\theta}_2 \in R^{(N-m-1)}$. Now from condition (C2), $\frac{1}{N}\mathbf{f}_N^\top\mathbf{f}_N \le \alpha^2$, we have

$$\frac{1}{N}\mathbf{f}_N^\top\mathbf{f}_N = \frac{1}{N}\boldsymbol{\theta}_2^\top\mathbf{U}_2^\top\mathbf{U}_2\boldsymbol{\theta}_2 = \frac{1}{N}\boldsymbol{\theta}_2^\top\mathbf{V}_2\boldsymbol{\theta}_2 \le \alpha^2.$$

■

Proof of Theorem 1. From (9), we have

$$\mathrm{MSE}(\hat{\boldsymbol{\theta}}_1, \mathbf{Z}_1, \boldsymbol{\theta}_2) = \sigma^2(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1} + (\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\boldsymbol{\theta}_2\boldsymbol{\theta}_2^\top\mathbf{Z}_2^\top\mathbf{Z}_1(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1},$$

and

$$
\begin{aligned}
\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1) &= \max_{\frac{1}{N}\boldsymbol{\theta}_2^\top \mathbf{V}_2\boldsymbol{\theta}_2\le\alpha^2} \det(\mathrm{MSE}(\hat{\boldsymbol{\theta}}_1, \mathbf{Z}_1, \boldsymbol{\theta}_2))\\
&= \max_{\frac{1}{N}\boldsymbol{\theta}_2^\top \mathbf{V}_2\boldsymbol{\theta}_2\le\alpha^2} \sigma^{2(m+1)} \det((\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1})(1+\frac{1}{\sigma^2}\boldsymbol{\theta}_2^\top\mathbf{Z}_2^\top\mathbf{Z}_1(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\boldsymbol{\theta}_2)\\
&= \sigma^{2(m+1)}\det((\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1})(1+\frac{N\alpha^2}{\sigma^2}\lambda_{\max}(\mathbf{A})),
\end{aligned}
$$

where $\mathbf{A} = \mathbf{V}_2^{-1/2}\mathbf{Z}_2^\top\mathbf{Z}_1(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\mathbf{V}_2^{-1/2}$, and $\lambda_{\max}(\mathbf{A})$ is the largest eigenvalue of $\mathbf{A}$.

Define

$$
\mathbf{W}_1 = \mathbf{U}_1\mathbf{V}_1^{-1/2}, \quad \mathbf{W}_2 = \mathbf{U}_2\mathbf{V}_2^{-1/2}.
$$

Since the columns of $\mathbf{U} = (\mathbf{U}_1, \mathbf{U}_2)$ are orthogonal, that is, $\mathbf{U}^\top\mathbf{U} = \mathbf{V}_1 \oplus \mathbf{V}_2$, we have

$$
\begin{aligned}
(\mathbf{W}_1, \mathbf{W}_2)^\top(\mathbf{W}_1, \mathbf{W}_2) &= \mathbf{I}_N,\\
(\mathbf{W}_1, \mathbf{W}_2)(\mathbf{W}_1, \mathbf{W}_2)^\top &= \mathbf{I}_N,
\end{aligned}
$$

where $\mathbf{I}_N$ is the $N \times N$ identity matrix.

A design ξ_n selected without replacement from design space $\mathbf{S}$ can be represented through a frequency vector $\mathbf{n}$ defined as $(n_1, \ldots, n_N)$, where $n_i = 0$ or 1. If point $\mathbf{s}_i$ is in ξ_n, then $n_i = 1$ otherwise 0. It is obvious that $\sum_{i=1}^N n_i = n$. Define an $N \times N$ diagonal matrix $\mathbf{M} = \mathrm{diag}\{n_1, \ldots, n_N\}$, then it is easy to verify that

$$
\begin{aligned}
\mathbf{Z}_1^\top\mathbf{Z}_1 &= \mathbf{U}_1^\top\mathbf{M}\mathbf{U}_1 = \mathbf{V}_1^{1/2}\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_1\mathbf{V}_1^{1/2},\\
\mathbf{Z}_1^\top\mathbf{Z}_2 &= \mathbf{U}_1^\top\mathbf{M}\mathbf{U}_2 = \mathbf{V}_1^{1/2}\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_2\mathbf{V}_2^{1/2}.
\end{aligned}
$$

Now

$$
\begin{aligned}
\lambda_{\max}(\mathbf{A}) &= \lambda_{\max}(\mathbf{V}_2^{-1/2}\mathbf{Z}_2^\top\mathbf{Z}_1(\mathbf{Z}_1^\top\mathbf{Z}_1)^{-1}\mathbf{Z}_1^\top\mathbf{Z}_2\mathbf{V}_2^{-1/2})\\
&= \lambda_{\max}(\mathbf{W}_2^\top\mathbf{M}\mathbf{W}_1(\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_1)^{-1}\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_2)\\
&= \lambda_{\max}((\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_1)^{-1}\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_2\mathbf{W}_2^\top\mathbf{M}\mathbf{W}_1)\\
&= \lambda_{\max}((\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_1)^{-1}\mathbf{W}_1^\top\mathbf{M}(\mathbf{I}-\mathbf{W}_1\mathbf{W}_1^\top)\mathbf{M}\mathbf{W}_1),\\
&= \lambda_{\max}(\mathbf{I}-\mathbf{W}_1^\top\mathbf{M}\mathbf{W}_1), \quad \text{using } \mathbf{M}^2 = \mathbf{M},\\
&= \lambda_{\max}(\mathbf{I}-\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2})\\
&= 1-\lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2}).
\end{aligned}
$$

Putting this result of $\lambda_{\max}(\mathbf{A})$ in $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$, we get the result in (11). ■

Proof of Theorem 2. From Theorem 1, a D-optimal minimax design for (13) minimizes loss function $\mathcal{L}_{\mathrm{D}}(\tilde{\mathbf{Z}}_1)$, which equals to

$$
\mathcal{L}_{\mathrm{D}}(\tilde{\mathbf{Z}}_1) = \sigma^{2(m+1)}\frac{1+\frac{N\alpha^2}{\sigma^2}(1-\lambda_{\min}(\tilde{\mathbf{V}}_1^{-1/2}\tilde{\mathbf{Z}}_1^\top\tilde{\mathbf{Z}}_1\tilde{\mathbf{V}}_1^{-1/2}))}{\det(\tilde{\mathbf{Z}}_1^\top\tilde{\mathbf{Z}}_1)}.
$$

From (12) and (13), we get

$$\begin{aligned}
\mathcal{L}_{\mathrm{D}}(\tilde{\mathbf{Z}}_1) &= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{B}_1^{-1}\mathbf{B}_1\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{B}_1\mathbf{B}_1^{-1}\mathbf{V}_1^{-1/2}))}{\det(\mathbf{B}_1\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{B}_1)} \\
&= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2}))}{\det(\mathbf{Z}_1^\top\mathbf{Z}_1)\prod_{i=1}^m b_i^2} \\
&= \frac{\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)}{\prod_{i=1}^m b_i^2}.
\end{aligned}$$

Since $\mathbf{Z}_1^*$ is a D-optimal minimax design for (7), it minimizes $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1)$. Thus $\tilde{\mathbf{Z}}_1^* = \mathbf{Z}_1^*\mathbf{B}_1$ minimizes $\mathcal{L}_{\mathrm{D}}(\tilde{\mathbf{Z}}_1)$ and is a D-optimal minimax design for (13). ■

Proof of Theorem 3. Since $\bar{\mathbf{u}}_j = q_j\mathbf{u}_j$ with $q_j = \pm 1$, $\|\bar{\mathbf{u}}_j\| = \|\mathbf{u}_j\| = l_i$. Notice that $\mathbf{Q}_1$ is a diagonal matrix, and $\mathbf{Q}_1^2 = \mathbf{I}$. From Theorem 1, we have

$$\begin{aligned}
\mathcal{L}_{\mathrm{D}}(\bar{\mathbf{Z}}_1) &= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\bar{\mathbf{Z}}_1^\top\bar{\mathbf{Z}}_1\mathbf{V}_1^{-1/2}))}{\det(\bar{\mathbf{Z}}_1^\top\bar{\mathbf{Z}}_1)} \\
&= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Q}_1\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{Q}_1\mathbf{V}_1^{-1/2}))}{\det(\mathbf{Q}_1\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{Q}_1)} \\
&= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{Q}_1\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2}\mathbf{Q}_1))}{\det(\mathbf{Q}_1\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{Q}_1)} \\
&= \sigma^{2(m+1)} \frac{1 + \frac{N\alpha^2}{\sigma^2}(1 - \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_1^\top\mathbf{Z}_1\mathbf{V}_1^{-1/2}))}{\det(\mathbf{Z}_1^\top\mathbf{Z}_1)} \\
&= \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1).
\end{aligned}$$

■

Proof of Theorem 4. To indicate that $\mathbf{Z}_1^*$ depends on run size n, we use notation $\mathbf{Z}_{1,n}^*$ for the D-optimal minimax design and $\mathbf{Z}_{1,n}$ for any design of size n. When the run size is $n+1$, we consider a design $\mathbf{Z}_{1,(n+1)}$ consisting of n runs from the D-optimal minimax design $\mathbf{Z}_{1,n}^*$ and one run at another design point in $\mathbf{S}$, say $\mathbf{s}_{n+1}$. Then

$$\mathbf{Z}_{1,(n+1)}^\top\mathbf{Z}_{1,(n+1)} = \mathbf{Z}_{1,n}^{*\ \top}\mathbf{Z}_{1,n}^* + \mathbf{s}_{n+1}\mathbf{s}_{n+1}^\top.$$

It is obvious that $\mathbf{Z}_{1,(n+1)}^\top\mathbf{Z}_{1,(n+1)} - \mathbf{Z}_{1,n}^{*\ \top}\mathbf{Z}_{1,n}^*$ is a positive semidefinite matrix. Thus $\det(\mathbf{Z}_{1,(n+1)}^\top\mathbf{Z}_{1,(n+1)}) \geq \det(\mathbf{Z}_{1,n}^{*\ \top}\mathbf{Z}_{1,n}^*)$. Also $\mathbf{V}_1^{-1/2}\mathbf{Z}_{1,(n+1)}^\top\mathbf{Z}_{1,(n+1)}\mathbf{V}_1^{-1/2} - \mathbf{V}_1^{-1/2}\mathbf{Z}_{1,n}^{*\ \top}\mathbf{Z}_{1,n}^*\mathbf{V}_1^{-1/2}$ is a positive semidefinite matrix, so we have $\lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_{1,(n+1)}^\top\mathbf{Z}_{1,(n+1)}\mathbf{V}_1^{-1/2}) \geq \lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{Z}_{1,n}^{*\ \top}\mathbf{Z}_{1,n}^*\mathbf{V}_1^{-1/2})$. Therefore $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_{1,n}^*) \geq \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_{1,(n+1)}) \geq \mathcal{L}_{\mathrm{D}}(\mathbf{Z}_{1,(n+1)}^*)$, which implies that $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^*)$ is a decreasing function of run size n.

When $n = N$, we have $\mathbf{Z}_1^* = \mathbf{U}_1$. Since $\mathbf{U}_1^\top\mathbf{U}_1 = \mathbf{V}_1$, $\lambda_{\min}(\mathbf{V}_1^{-1/2}\mathbf{U}_1^\top\mathbf{U}_1\mathbf{V}_1^{-1/2}) = 1$ and $\det(\mathbf{U}_1^\top\mathbf{U}_1) = \det(\mathbf{V}_1) = N\prod_{i=1}^m l_i^2$. Hence $\mathcal{L}_{\mathrm{D}}(\mathbf{Z}_1^*) = \sigma^{2(m+1)}/(N\prod_{i=1}^m l_i^2)$. ■

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