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A class of space-filling designs and their projection properties

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A B S T R A C T

This paper introduces a class of transformation-based metrics, and uses them to construct maximin-type, minimax-type, and ϕ_p-type designs. The proposed designs include many distance-based designs as special cases. Theoretical and numerical results are presented to show the relationship between projection properties of such a design and the transformation used in it.

1. Introduction

A set of points $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is called a space-filling design (Santner et al., 2003) in the experimental region $\mathcal{X} \subset \mathbb{R}^d$ if it scatters the points uniformly over $\mathcal{X}$, where $\mathbf{x}_i = (x_{i1}, \ldots, x_{id})'$ for $i = 1, \ldots, n$. Many space-filling criteria have been proposed, mostly based on a distance or metric on $\mathcal{X}$. For example, let $\|\cdot\|$ denote the Euclidean norm. A popular criterion is the minimum distance criterion

$$\mathrm{m}(D) = \mathrm{m}(\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}) = \min_{1\leqslant i<j\leqslant n} \|\mathbf{x}_i - \mathbf{x}_j\|, \tag{1}$$

and the maximin distance design (Johnson et al., 1990) is the solution that maximizes this criterion. The minimization operation in (1) is not differentiable, and this may cause difficulties in optimizing it. A smooth modification of (1) is the ϕ_p criterion (Morris and Mitchell, 1995) $\phi_p(D) = \left(\sum_{1\leqslant i<j\leqslant n} \|\mathbf{x}_i - \mathbf{x}_j\|^{-p}\right)^{1/p}$. A design that minimizes the ϕ_p criterion tends to the maximin distance design as $p \to \infty$. Another common space-filling criterion based on the Euclidean norm is the maximum distance criterion $\mathrm{M}(D) = \max_{\mathbf{x}\in\mathcal{X}} \min_{\mathbf{x}_i\in D} \|\mathbf{x} - \mathbf{x}_i\|$, and the minimax distance design (Johnson et al., 1990) is the solution that minimizes M.

Besides the space-filling property, uniformity in projection spaces of the experimental region is also appealing. Some authors optimized the above space-filling criteria within the class of Latin hypercube designs (LHDs McKay et al., 1979) to guarantee the one-dimensional projection property (Park, 2001; Morris and Mitchell, 1995). Draguljic et al. (2012) and Mu and Xiong (2017) proposed criteria to handle all the one to d-dimensional projection spaces. However, their criteria are too complicated to optimize. Recently, Joseph et al. (2015) proposed the criterion $\psi(D) = \left[\sum_{1\leqslant i<j\leqslant n} \left\{\prod_{l=1}^{d} (x_{il} - x_{jl})\right\}^{-2}\right]^{1/d}$, and called the solution minimizing ψ the maximum projection design. This criterion takes all projection spaces into account, and can be optimized at no more cost than the minimum distance criterion or ϕ_p criterion.

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Based on coordinate-wise transformations, this paper introduces a broad class of metrics (quasi-distances) on $\mathbb{R}^d$, and uses them to construct maximin-type, minimax-type, and ϕ_p-type designs. We next focus on the designs in which the coordinate-wise transformation is the Box–Cox transformation (Box and Cox, 1964) with parameter λ. The maximin distance design and maximum projection design are two special cases of such designs corresponding to $\lambda = 1$ and $\lambda = 0$, respectively. Theoretical and numerical results are presented to show the relationship between projection properties of the designs and λ. In particular, for sufficiently small λ ($\to -\infty$), the proposed maximin-type designs achieve uniformity in one-dimensional projection spaces, and then belong to LHDs, and this result constructs a connection between distance-based space-filling designs and LHDs. We conclude that the proposed designs provide abundant choices of space-filling designs with different projection properties.

2. Designs based on coordinate-transform metrics

Let g be an increasing transformation on $[0, +\infty)$, and $g(0) = g(0+)$ can be $-\infty$.

Definition 1. For $\mathbf{a} = (a_1, \ldots, a_d)'$, $\mathbf{b} = (b_1, \ldots, b_d)'$, define the coordinate-transform metric between $\mathbf{a}$ and $\mathbf{b}$ with respect to g as

$$\rho_g(\mathbf{a}, \mathbf{b}) = \sum_{j=1}^{d} g\big((a_j - b_j)^2\big). \tag{2}$$

By replacing the Euclidean norm in the criteria in Section 1 by ρ_g, we can obtain a number of design criteria. First, like (1), the minimum ρ_g criterion is

$$\mathrm{m}_g(D) = \mathrm{m}_g(\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}) = \min_{1\leqslant i<j\leqslant n} \rho_g(\mathbf{x}_i, \mathbf{x}_j), \tag{3}$$

and then the maximin ρ_g design is the solution that maximizes this criterion. Similarly, we can define minimax ρ_g design as the solution that minimizes $\mathrm{M}_g(D) = \max_{\mathbf{x}\in\mathcal{X}} \min_{i=1,\ldots,n} \rho_g(\mathbf{x}, \mathbf{x}_i)$. To extend the ϕ_p criterion, we need an increasing function h valued in $[0, +\infty)$. Based on ρ_g and h, a general $\phi_{g,h}$ criterion is

$$\phi_{g,h}(D) = \sum_{1\leqslant i<j\leqslant n} \frac{1}{\left[h\left(\rho_g(\mathbf{x}_i, \mathbf{x}_j)\right)\right]}. \tag{4}$$

The design minimizing (4) is called the minimum $\phi_{g,h}$ design. We can also get maximin ρ_g LHDs, minimax ρ_g LHDs, and minimum $\phi_{g,h}$ LHDs by optimizing these criteria within the class of LHDs.

Some choices of the transformation g in (2) are as follows.

(i). The identity transformation: $g(x) = x$, which implies $\rho_g(\mathbf{a}, \mathbf{b}) = \|\mathbf{a} - \mathbf{b}\|^2$. This coordinate-transform metric yields traditional maximin and minimax distance designs. For $h(x) = x^{p/2}$ in (4), we get the minimum ϕ_p design by minimizing (4).

(ii). The log transformation: $g(x) = \log(x)$. For $h(x) = \exp(x)$, minimization of (4) gives Joseph et al. (2015)'s maximum projection design.

(iii). The Box–Cox transformation: for $\lambda \in \mathbb{R}$,

$$g_\lambda(x) = \begin{cases} (x^\lambda - 1)/\lambda, & \lambda \neq 0; \\ \log(x), & \lambda = 0. \end{cases} \tag{5}$$

Clearly, the class includes (i) and (ii) as special cases. For $\lambda \geqslant 1/2$, the corresponding maximin and minimax ρ_g designs are actually maximin and minimax $\ell_{2\lambda}$ distance designs, respectively. Besides the ℓ_2 (Euclidean) distance, the minimum ℓ_1 distance criterion is sometimes used (Ye, Li, and Sudjianto 2000; van Dam et al. 2007).

3. Projection properties of ρ_g-based designs

This section considers how projection properties of a ρ_g-based design depend on the transformation g.

Definition 2. For a design $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset \mathcal{X} \subset \mathbb{R}^d$ and $s = 1, \ldots, d$, we say that D has the s-dimensional non-overlapping property if for all $i \neq j$ and $1 \leqslant l_1 < \cdots < l_s \leqslant d$, $(x_{il_1}, \ldots, x_{il_s})' \neq (x_{jl_1}, \ldots, x_{jl_s})'$.

The s-dimensional non-overlapping property implies the s'-dimensional non-overlapping property for all $s' > s$. The non-overlapping property guarantees the uniformity in projection spaces at the lowest level. In other words, a design that does not have the s-dimensional non-overlapping property cannot scatter the points uniformly in s' dimensions for all $s' \leqslant s$. It is easy to obtain the following theorem.

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