The Canadian Journal of Statistics
Vol. 51, No. 1, 2023, Pages 293–311
La revue canadienne de statistique

Two-dimensional projection uniformity for space-filling designs

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Key words and phrases: Computer experiment; discrepancy; Latin hypercube; maximin distance; uniform projection design.

MSC 2020: Primary 62K15; secondary 62K99.

Abstract: We investigate a space-filling criterion based on L_2-type discrepancies, namely the uniform projection criterion, aiming at improving designs' two-dimensional projection uniformity. Under a general reproducing kernel, we establish a formula for the uniform projection criterion function, which builds a connection between rows and columns of the design. For the commonly used discrepancies, we further use this formula to represent the two-dimensional projection uniformity in terms of the L_p-distances of U-type designs. These results generalize existing works and reveal new links between the two seemingly unrelated criteria of projection uniformity and the maximin L_p-distance for U-type designs. We also apply the obtained results to study several families of space-filling designs with appealing projection uniformity. Because of good projected space-filling properties, these designs are well adapted for computer experiments, especially for the case where not all the input factors are active. *The Canadian Journal of Statistics* 51: 293–311; 2023 © 2022 Statistical Society of Canada

Résumé: Nous étudions un critère de remplissage d'espace basé sur des écarts de type L_2, à savoir le critère de projection uniforme, et ce dans le but d'améliorer l'uniformité des plans de projection en deux dimensions. En travaillant dans le cadre d'un noyau autoreproduisant général, nous présentons une expression du critère de projection uniforme qui établit un lien entre les lignes et les colonnes du plan. Pour les écarts couramment utilisés, nous utilisons en outre cette formule pour exprimer l'uniformité de la projection bidimensionnelle en termes de distances L_p pour des plans de type U. Ces résultats généralisent les travaux existants et révèlent de nouveaux liens entre deux critères sans lien apparent, celui de la projection uniforme et celui du maximin de distances L_p dans des plans de type U. Nous appliquons également les résultats obtenus pour étudier plusieurs familles de plans d'expérience comblant l'espace ayant une uniformité de projection intéressante. En raison des bonnes propriétés des projections obtenues, ces plans sont bien adaptés aux expériences sur ordinateur, en particulier pour le cas où tous les facteurs d'entrée ne sont pas actifs. *La revue canadienne de statistique* 51: 293–311; 2023 © 2022 Société statistique du Canada

1. INTRODUCTION

Space-filling designs have been increasingly applied in computer and physical experiments for studying complex systems (Santner, Williams & Notz, 2003; Fang, Li & Sudjianto, 2006; Lin & Tang, 2015). A widely used class of space-filling designs is uniform designs (Fang et al., 2018), which also play a crucial role in quasi-Monte Carlo methods. Let (n, s^m) denote an n-run design

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with m factors, each taking s levels from the set $\mathcal{Z}_s = \{0, 1, \dots, s-1\}$. Such a design can be represented by an $n \times m$ matrix $D = (x_{ik})$, where $x_{ik} \in \mathcal{Z}_s$ is the (i, k)th entry, $1 \le i \le n$, $1 \le k \le m$. A uniform design D attempts to scatter its n points as evenly as possible over the design space by minimizing a measure called discrepancy.

There are various discrepancy metrics proposed from different considerations. Roughly speaking, a discrepancy defines a measure of the difference between the empirical distribution of D and the uniform distribution over the design space. Using a method of reproducing kernel Hilbert spaces, researchers have proposed several popular L_2-type discrepancies (Hickernell, 1998a, 1998b; Hickernell & Liu, 2002; Zhou, Fang & Ning, 2013) including the (modified) L_2-star discrepancy, the centred L_2-discrepancy (CD), the symmetric L_2-discrepancy (SD), the wrap-around L_2-discrepancy (WD), and the mixture discrepancy (MD). Without loss of generality, suppose the experimental domain is the unit hypercube $[0, 1]^m$. For an (n, s^m) design $D = (x_{ik})$, we rescale the design points into the region $[0, 1]^m$ through the mapping $x_{ik} \mapsto (2x_{ik} + 1)/(2s)$. Let $K(x, y)$ be a reproducing kernel defined on $[0, 1]^m \times [0, 1]^m$ with a multiplicative form

$$K(x, y) = \prod_{k=1}^{m} f(x_k, y_k), \quad f : [0, 1]^2 \to \mathbb{R}. \tag{1}$$

Then, by Hickernell (1998a) and Zhou & Xu (2014), for a design D, its L_2-type discrepancy induced by the kernel $K(x, y)$ has the general expression

$$\begin{aligned} \mathrm{Disc}(D, K) = {} & \left[\iint_{[0,1]^2} f(x, y)dxdy\right]^m - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(\int_0^1 f\left(\frac{2x_{ik}+1}{2s}, y\right)dy\right) \\ & + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m} f\left(\frac{2x_{ik}+1}{2s}, \frac{2x_{jk}+1}{2s}\right). \end{aligned} \tag{2}$$

A design D is called a uniform design under the discrepancy (2) if it has the minimum $\mathrm{Disc}(D, K)$ value among all (n, s^m) designs.

As observed by Zhou, Fang & Ning (2013), commonly used discrepancies such as the CD have a dimensionality effect which tends to put more points close to the centre point in the whole dimensional space as the dimension becomes high. A uniform design might prioritize uniformity among the overall and high-dimensional projections but have bad low-dimensional projections. In practice, the response of a system is usually dominated by main effects and low-order interactions. Under such an effect sparsity scenario, the projection properties of a design are more important. A good design should focus more on the space-filling properties in its low-dimensional projections (Santner, Williams & Notz, 2003; Moon, Dean & Santner, 2012; Woods & Lewis, 2016). Using this idea, the MaxPro designs (Joseph, Gul & Ba, 2015), minimax projection designs (Mak & Joseph, 2018), and uniform projection designs (Sun, Wang & Xu, 2019) have been recently proposed. Following the research line of Sun, Wang & Xu (2019), in this article, we systematically study the uniform projection criterion minimizing the average discrepancy for all two-dimensional projections of a design. We establish a general formula representing the uniform projection criterion by a measure of relationships between rows of the design. We then show the explicit connections between the uniform projection criteria and the L_p-distances of the design under the commonly used discrepancies. The obtained results not only reveal links between the two seemingly unrelated criteria of projection uniformity and the maximin L_p-distance but also inspire us to study and construct better space-filling designs.

The theory in this article generalizes the previous results in Sun, Wang & Xu (2019) and Wang, Sun & Xu (2020). In those two works, the authors consider only the uniform projection criterion based on the CD. Instead, we establish general results for any L_2-type discrepancies (2) and more elaborate results for the commonly used discrepancies. For example, the (modified) L_2-star discrepancy, the CD, and the SD are all special cases of an important class of L_2-type discrepancies called the generalized L_2-type discrepancy, which was proposed by Hickernell (1998a) using Bernoulli polynomials (see (9)). We show in Section 3.1 that the uniform projection criteria for all generalized L_2-type discrepancies are equivalent, resulting in a unified theory for the (modified) L_2-star discrepancy, the CD, and the SD.

The remainder of this article is organized as follows. In Section 2, we introduce some notations and then give a general representation formula for the uniform projection criteria. Based on this formula, in Section 3, we further explore the uniform projection criteria and their connections with the L_p-distances of designs under some commonly used discrepancies. In Section 4, we study the two-dimensional uniformity of several families of space-filling designs. Section 5 concludes the article with a discussion. The Supplementary Material includes some technical details and additional results.

2. UNIFORM PROJECTION CRITERION AND A GENERAL REPRESENTATION FORMULA

Let $D = (x_{ik})$ be an (n, s^m) design with $m \geq 2$. It is called a U-type design if the columns are balanced, that is, in each column, each of the s levels appears the same number of times. This means that n/s is an integer. More generally, D is called an orthogonal array of strength $t \geq 1$, denoted as $OA(n, s^m, t)$, if n/s^t is an integer and in each set of t-columns of D, all the level-combinations appear n/s^t times. A U-type design is an $OA(n, s^m, 1)$ and, in particular, a U-type (n, n^m) design is called a Latin hypercube design (LHD) and is denoted by $LHD(n, m)$ (McKay, Beckman & Conover, 1979). LHDs have been widely applied as computer experimental designs.

The uniform projection criterion was proposed by Sun, Wang & Xu (2019) to improve the low-dimensional projection properties of a design by minimizing the average CD of all two-dimensional projections of the design. Here we generalize the uniform projection criterion to an arbitrary L_2-type discrepancy defined in (2) as

$$\Phi_{\text{Disc}}(D) = \frac{2}{m(m-1)} \sum_{|u|=2} \text{Disc}(D_u, K), \tag{3}$$

where u is a subset of $\{1, 2, \ldots, m\}$, $|u|$ denotes the cardinality of u, and D_u is the projected design of an (n, s^m) design D onto dimensions indexed by the elements of u. We call an (n, s^m) design D a uniform projection design under the discrepancy (2) if it has the minimum Φ_{Disc} value among all (n, s^m) designs.

The following proposition shows that the average Φ_{Disc} value of all k-factor ($k \geq 2$) projected designs is still Φ_{Disc}. Therefore, a uniform projection design tends to have small $\Phi_{\text{Disc}}(D_u)$ values for all projections. The proof is straightforward and omitted.

Proposition 1. *Let D be a U-type (n, s^m) design. For any $2 \leq k \leq m$,*

$$\frac{1}{\binom{m}{k}} \sum_{|u|=k} \Phi_{\text{Disc}}(D_u) = \Phi_{\text{Disc}}(D),$$

where D_u is the projected design onto k factors indexed by u.

By the definition (3), to obtain a design's Φ_{Disc} value, we first calculate the discrepancies of all the column pairwise projections of D and then take an average. Therefore, (3) can be viewed as a measure of a design's column pairwise relationships. Theorem 1 establishes a new formula of (3) for U-type designs from a viewpoint of row pairwise relationships.

Theorem 1. *For a U-type (n, s^m) design $D = (x_{ik})$,*

$$\Phi_{\text{Disc}}(D) = \frac{F_{\text{Disc}}(D)}{n^2 m(m-1)} + C_{\text{Disc}}(m, s), \tag{4}$$

where

$$F_{\text{Disc}}(D) = \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sum_{k=1}^{m} f\left(\frac{2x_{ik}+1}{2s}, \frac{2x_{jk}+1}{2s}\right)\right)^2 - 2n\sum_{i=1}^{n}\left(\sum_{k=1}^{m}\int_0^1 f\left(\frac{2x_{ik}+1}{2s}, y\right)dy\right)^2 \tag{5}$$

and

$$C_{\text{Disc}}(m, s) = \left(\int_{[0,1]^2} f(x,y)dxdy\right)^2 + \frac{2}{(m-1)s}\sum_{i=0}^{s-1}\left(\int_0^1 f\left(\frac{2i+1}{2s}, y\right)dy\right)^2 - \frac{1}{(m-1)s^2}\sum_{i=0}^{s-1}\sum_{j=0}^{s-1} f\left(\frac{2i+1}{2s}, \frac{2j+1}{2s}\right)^2 \tag{6}$$

is a constant only determined by m, s, and the kernel function $f(\cdot,\cdot)$.

Proof of Theorem 1. For any U-type (n, s^m) design $D = (x_{ik})$, let G_1 and G_2, respectively, denote the following two terms:

$$\sum_{1\le k_1<k_2\le m}\sum_{i=1}^{n}\left(\int_0^1 f\left(\frac{2x_{ik_1}+1}{2s}, y\right)dy\right)\left(\int_0^1 f\left(\frac{2x_{ik_2}+1}{2s}, y\right)dy\right)$$

and

$$\sum_{1\le k_1<k_2\le m}\sum_{i=1}^{n}\sum_{j=1}^{n} f\left(\frac{2x_{ik_1}+1}{2s}, \frac{2x_{jk_1}+1}{2s}\right) f\left(\frac{2x_{ik_2}+1}{2s}, \frac{2x_{jk_2}+1}{2s}\right).$$

Then we can represent (3) as

$$\Phi_{\text{Disc}}(D) = \frac{2}{n^2 m(m-1)}G_2 - \frac{4}{nm(m-1)}G_1 + \left(\int_{[0,1]^2} f(x,y)dxdy\right)^2. \tag{7}$$

Let $g_k^i = \int_0^1 f\left(\frac{2x_{ik}+1}{2s}, y\right)dy$. Then

$$\begin{aligned} G_1 &= \sum_{i=1}^{n}\sum_{1\le k_1<k_2\le m} g_{k_1}^i g_{k_2}^i \\ &= \sum_{i=1}^{n}\frac{1}{2}\left[\left(g_1^i + \cdots + g_m^i\right)^2 - \left((g_1^i)^2 + \cdots + (g_m^i)^2\right)\right] \end{aligned}$$

$$= \frac{1}{2}\sum_{i=1}^{n}\left(\sum_{k=1}^{m}\int_0^1 f\left(\frac{2x_{ik}+1}{2s}, y\right)dy\right)^2 - \frac{m}{2}\sum_{i=1}^{n}\left(g_1^i\right)^2$$

$$= \frac{1}{2}\sum_{i=1}^{n}\left(\sum_{k=1}^{m}\int_0^1 f\left(\frac{2x_{ik}+1}{2s}, y\right)dy\right)^2 - \frac{nm}{2s}\sum_{i=0}^{s-1}\left(\int_0^1 f\left(\frac{2i+1}{2s}, y\right)dy\right)^2.$$

Similarly, let $h_k^{ij} = f\left(\frac{2x_{ik}+1}{2s}, \frac{2x_{jk}+1}{2s}\right)$; we have

$$G_2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{1\le k_1<k_2\le m} h_{k_1}^{ij}h_{k_2}^{ij}$$

$$= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left[\left(h_1^{ij}+\cdots+h_m^{ij}\right)^2 - \left(\left(h_1^{ij}\right)^2+\cdots+\left(h_m^{ij}\right)^2\right)\right]$$

$$= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sum_{k=1}^{m} f\left(\frac{2x_{ik}+1}{2s}, \frac{2x_{jk}+1}{2s}\right)\right)^2 - \frac{m}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(h_1^{ij}\right)^2$$

$$= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sum_{k=1}^{m} f\left(\frac{2x_{ik}+1}{2s}, \frac{2x_{jk}+1}{2s}\right)\right)^2 - \frac{n^2m}{2s^2}\sum_{i=0}^{s-1}\sum_{j=0}^{s-1} f\left(\frac{2i+1}{2s}, \frac{2j+1}{2s}\right)^2.$$

The desired result follows by substituting G_1 and G_2 into (7) and simplifying. ■

Theorem 1 represents the projection uniformity by a new space-filling measure of rows, that is, the function $F_{\text{Disc}}(D)$ defined in (5). Minimizing $\Phi_{\text{Disc}}(D)$ is equivalent to minimizing $F_{\text{Disc}}(D)$ in (5). As a result, Theorem 1 establishes a link between the relationships of rows and columns of the design.

In the next section, we take a closer look at the generalized L_2-discrepancy (which covers the (modified) L_2-star discrepancy, the CD, and the SD), the WD, and the MD, respectively, to connect projection uniformity under these commonly used discrepancies with the L_p-distances of the design.

3. RESULTS FOR THE COMMONLY USED DISCREPANCIES

3.1. Generalized L_2-discrepancy

Let $\mu(\cdot)$ be any arbitrary one-dimensional function satisfying $\int_0^1 \mu(x)dx = 0$ and $\int_0^1 \left(\frac{d\mu}{dx}\right)^2 dx < \infty$, and let β be some arbitrary positive constant. For an (n, s^m) design $D = (x_{ik})$, we take the kernel function in (1) to be

$$f(x,y) = M + \beta^2\left(\mu(x)+\mu(y)+\frac{1}{2}B_2(\{x-y\}) + B_1(x)B_1(y)\right), \tag{8}$$

where $B_1(x) = x - 1/2$ and $B_2(x) = x^2 - x + 1/6$ are Bernoulli polynomials of orders 1 and 2, respectively; $\{x\} = x - \lfloor x \rfloor$, $\lfloor x \rfloor$ is the largest integer not exceeding x; and $M = 1 + \beta^2\int_0^1\left(\frac{d\mu}{dx}\right)^2 dx$.

Then the (squared) generalized L_2-discrepancy (abbreviated as GD) of D, proposed by Hickernell (1998a), is defined as

$$\begin{aligned}\mathrm{GD}(D) = M^m &- \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(M + \beta^2\mu\left(\frac{2x_{ik}+1}{2s}\right)\right)\\ &+ \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(M + \beta^2\left[\mu\left(\frac{2x_{ik}+1}{2s}\right)\right.\right.\\ &+ \mu\left(\frac{2x_{jk}+1}{2s}\right) + \frac{1}{2}B_2\left(\left\{\frac{2x_{ik}-2x_{jk}}{2s}\right\}\right)\\ &\left.\left.+ B_1\left(\frac{2x_{ik}+1}{2s}\right)B_1\left(\frac{2x_{jk}+1}{2s}\right)\right]\right). \qquad (9)\end{aligned}$$

Next, we will link the uniform projection criterion $\Phi_{\mathrm{GD}}(D)$ with the distances between rows of $D = (x_{ik})$. The L_p-distance between the ith row $x_i = (x_{i1}, \ldots, x_{im})$ and the jth row $x_j = (x_{j1}, \ldots, x_{jm})$ in D is defined as

$$d_p(x_i, x_j) = \sum_{k=1}^{m}|x_{ik} - x_{jk}|^p, \qquad (10)$$

which takes the pth power of the standard L_p-distance for convenience. The minimum L_p-distance of a design D is defined to be $d_p(D) = \min_{1\le i<j\le n} d_p(x_i, x_j)$. The maximin distance criterion is a widely used space-filling criterion which was proposed by Johnson, Moore & Ylvisaker (1990). An (n, s^m) design D is called a maximin L_p-distance design if it maximizes the $d_p(D)$ value among all (n, s^m) designs. In practice, the most commonly used distances are the L_1-(Manhattan) and L_2-(Euclidean) distances. One formal justification of maximin distance designs given in Johnson, Moore & Ylvisaker (1990) is that maximin distance designs are asymptotically D-optimal under the ordinary kriging model as the correlations become weak.

For any U-type (n, s^m) design D, the average pairwise L_p-distance, denoted as $\bar{d}_p = \sum_{1\le i<j\le n} d_p(x_i, x_j)/\binom{n}{2}$, is always a constant. Specifically,

$$\bar{d}_1 = \frac{nm(s^2-1)}{3(n-1)s} \quad \text{and} \quad \bar{d}_2 = \frac{nm(s^2-1)}{6(n-1)}. \qquad (11)$$

Zhou & Xu (2015) established the following upper bounds:

Lemma 1. *For a U-type (n, s^m) design $D = (x_{ik})$, $d_1(D) \le \lfloor \bar{d}_1 \rfloor$, and $d_2(D) \le \lfloor \bar{d}_2 \rfloor$.*

The following theorem represents $\Phi_{\mathrm{GD}}(D)$ as a function of the pairwise L_1-distances between design points in D.

Theorem 2. *For a U-type (n, s^m) design $D = (x_{ik})$,*

$$\Phi_{\mathrm{GD}}(D) = \frac{\beta^4 g_{\mathrm{GD}}(D)}{4n^2m(m-1)s^2} + \tilde{C}_{\mathrm{GD}}(m, s), \qquad (12)$$

 DOI: 10.1002/cjs.11686

where

$$g_{\mathrm{GD}}(D) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_1^2(x_i, x_j) - \frac{2}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{n} d_1(x_i, x_j)\right)^2, \tag{13}$$

$d_1(x_i, x_j)$ is the L_1-distance between x_i and x_j defined in (10), and

$$\begin{aligned}\tilde{C}_{\mathrm{GD}}(m,s) = {} & \frac{\beta^4}{3s^3}\mu_1 + \frac{2\beta^4}{s^2}\mu_1^2 + \frac{M\beta^2}{6s^2} + \frac{\beta^4}{36} - \frac{\beta^4}{18s^2} + \frac{5\beta^4}{144s^4} \\ & + \frac{1}{m-1}\left[\left(-\frac{\beta^4}{2s} + \frac{\beta^4}{2s^3}\right)\mu_1 - \frac{\beta^4}{2s^3}\mu_2 + \frac{2\beta^4}{s^3}\mu_3 + \left(\frac{\beta^4}{60} - \frac{\beta^4}{12s^2} + \frac{\beta^4}{15s^4}\right)\right]\end{aligned}$$

with

$$\mu_1 = \sum_{l=0}^{s-1}\mu\left(\frac{2l+1}{2s}\right), \mu_2 = \sum_{l=0}^{s-1}\mu\left(\frac{2l+1}{2s}\right)(2l-s+1)^2, \mu_3 = \sum_{i=0}^{s-1}\sum_{j=0}^{s-1}\mu\left(\frac{2i+1}{2s}\right)|i-j|.$$

Proof of Theorem 2. Let μ_1, μ_2, μ_3 be the constants defined above, and $\mu_4 = \sum_{l=0}^{s-1}\mu\left(\frac{2l+1}{2s}\right)^2$. We now apply Theorem 1 to get Theorem 2. For $D = (x_{ik})$, let $z_{ik} = (2x_{ik} - s + 1)/(2s)$. Denote $\alpha_i = \sum_{k=1}^{m}\mu\left(z_{ik} + \frac{1}{2}\right)$ and $s_0 = (s-1)/2$. Using the facts that $d_2(z_i, 0) = d_2(x_i, s_0)/s^2$ and $d_1(z_i, z_j) = d_1(x_i, x_j)/s$, and Lemmas 2 and 3 in the Supplementary Material, we have that the term $F_{\mathrm{Disc}}(D)$ defined in (5) in Theorem 1 equals

$$\begin{aligned}F_{\mathrm{GD}}(D) &= \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sum_{k=1}^{m} f\left(z_{ik} + \frac{1}{2}, z_{jk} + \frac{1}{2}\right)\right)^2 - 2n\sum_{i=1}^{n}\left(\sum_{k=1}^{m}\int_0^1 f\left(z_{ik} + \frac{1}{2}, y\right)dy\right)^2 \\ &= \beta^4\left(\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\alpha_i + \alpha_j + \frac{d_2(z_i,0)}{2} + \frac{d_2(z_j,0)}{2} - \frac{d_1(z_i,z_j)}{2}\right)^2 - 2n\sum_{i=1}^{n}\alpha_i^2\right) \\ &\quad + n^2m^2\left(M + \frac{\beta^2}{12}\right)^2 - \frac{n^2m^2(s^2-1)\left(M + \frac{\beta^2}{12}\right)\beta^2}{6s^2} \\ &\quad + \frac{4n^2m^2\left(M + \frac{\beta^2}{12}\right)\beta^2}{s}\mu_1 - 2n^2m^2M^2 - \frac{4n^2m^2M\beta^2}{s}\mu_1 \\ &= \frac{\beta^4}{4s^2}g_{\mathrm{GD}}(D) + n^2m^2\left(\frac{2\beta^4}{s^2}\mu_1^2 + \frac{\beta^4}{3s^3}\mu_1 - M^2 + \frac{M\beta^2}{6s^2} + \frac{\beta^4}{36} - \frac{\beta^4}{18s^2} + \frac{5\beta^4}{144s^4}\right),\end{aligned}$$

where $g_{\mathrm{GD}}(D)$ is defined in (13).

Besides, the term $\sum_{i=0}^{s-1}\left[\int_0^1 f((2i+1)/(2s), y)\,dy\right]^2$ in Theorem 1 equals

$$\sum_{i=0}^{s-1}\left(M + \beta^2\mu\left(\frac{2i+1}{2s}\right)\right)^2 = M^2 s + 2M\beta^2\mu_1 + \beta^4\mu_4$$

and the term $\sum_{i=0}^{s-1}\sum_{j=0}^{s-1}\left[f\left((2i+1)/(2s),(2j+1)/(2s)\right)\right]^2$ equals

$$\sum_{i=0}^{s-1}\sum_{j=0}^{s-1}\left(M+\frac{\beta^2}{12}+\beta^2\left[\mu\left(\frac{2i+1}{2s}\right)+\mu\left(\frac{2j+1}{2s}\right)+\frac{1}{2}\left|\frac{2i-s+1}{2s}\right|^2\right.\right.$$
$$\left.\left.+\frac{1}{2}\left|\frac{2j-s+1}{2s}\right|^2-\frac{1}{2}\left|\frac{i-j}{s}\right|\right]\right)$$
$$=\left(4M\beta^2 s+\frac{\beta^4 s}{2}-\frac{\beta^4}{6s}\right)\mu_1+2\beta^4\mu_1^2+\frac{\beta^4}{2s}\mu_2-\frac{2\beta^4}{s}\mu_3+2\beta^4 s\mu_4$$
$$+\left(M^2s^2+\frac{M\beta^2}{6}+\frac{\beta^4 s^2}{90}+\frac{\beta^4}{36}-\frac{23\beta^4}{720}\right).$$

Then the constant $C_{\mathrm{Disc}}(m,s)$ defined in (6) in Theorem 1 simplifies to

$$C_{\mathrm{GD}}(m,s)=M^2+\frac{1}{m-1}\left[\left(-\frac{\beta^4}{2s}+\frac{\beta^4}{6s^3}\right)\mu_1-\frac{2\beta^4}{s^2}\mu_1^2-\frac{\beta^4}{2s^3}\mu_2+\frac{2\beta^4}{s^3}\mu_3\right.$$
$$\left.+\left(M^2-\frac{M\beta^2}{6s^2}-\frac{\beta^4}{90}-\frac{\beta^4}{36s^2}+\frac{23\beta^4}{720s^4}\right)\right].$$

Finally, the desired result follows by combining the above equations and some algebra. ■

Theorem 2 shows that, regardless of the choice of $\mu(\cdot)$, M, and β in (8), the two-dimensional projection uniformity for all different GDs is only related to the L_1-distances of the design. The following three examples discuss the (modified) L_2-star discrepancy, the CD, and the SD, respectively.

Example 1 (The (modified) L_2-star discrepancy)**.** For an (n,s^m) design $D=(x_{ik})$, the (modified) L_2-star discrepancy (Hickernell, 1998a) is

$$\mathrm{D}_2^*(D)=\left(\frac{4}{3}\right)^m-\frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(\frac{3}{2}-\frac{1}{2}\left(\frac{2x_{ik}+1}{2s}\right)^2\right)$$
$$+\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(2-\max\left(\frac{2x_{ik}+1}{2s},\frac{2x_{jk}+1}{2s}\right)\right).$$

Following Hickernell (1998a), D_2^* is a special case of the GD with

$$\mu(x)=-\frac{x^2}{2}+\frac{1}{6},\quad \beta=1,\ \text{and}\ M=\frac{4}{3}.$$

Then by Lemma 2 in the Supplementary Material and some calculations

$$\mu_1=-\frac{1}{2}\sum_{i=0}^{s-1}\left|\frac{2i+1}{2s}\right|^2+\frac{s}{6}=\frac{1}{24s},$$

$$\mu_2 = -2s^2\sum_{i=0}^{s-1}\left|\frac{2i+1}{2s}\right|^2\left|\frac{2i+1-s}{2s}\right|^2 + \frac{2s^2}{3}\sum_{i=0}^{s-1}\left|\frac{2i+1-s}{2s}\right|^2 = -\frac{s^3}{90}+\frac{5s}{72}-\frac{7}{120s},$$

$$\mu_3 = -\frac{s}{2}\sum_{i=0}^{s-1}\sum_{j=0}^{s-1}\left|\frac{2i+1}{2s}\right|^2\left|\frac{i-j}{s}\right| + \frac{s}{6}\sum_{i=0}^{s-1}\sum_{j=0}^{s-1}\left|\frac{i-j}{s}\right| = -\frac{s^3}{360}+\frac{s}{36}-\frac{1}{40s}.$$

Hence,

$$\Phi_{\mathrm{D}_2^*}(D) = \frac{g_{\mathrm{D}_2^*}(D)}{4n^2m(m-1)s^2} + \tilde{C}_{\mathrm{D}_2^*}(m,s),$$

where $g_{\mathrm{D}_2^*}(D) = g_{\mathrm{GD}}(D)$ in (13) and

$$\tilde{C}_{\mathrm{D}_2^*}(m,s) = \left(\frac{1}{36}+\frac{1}{6s^2}+\frac{5}{96s^4}\right) + \frac{1}{m-1}\left(\frac{1}{60}-\frac{1}{12s^2}+\frac{1}{15s^4}\right).$$

Example 2 (The CD)**.** For an (n, s^m) design $D = (x_{ik})$

$$\mathrm{CD}(D) = \left(\frac{13}{12}\right)^m - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right| - \frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right|^2\right)$$
$$+\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right| + \frac{1}{2}\left|\frac{2x_{jk}+1-s}{2s}\right| - \frac{1}{2}\left|\frac{x_{ik}-x_{jk}}{s}\right|\right).$$

Following Hickernell (1998a), the CD is a special case of the GD with

$$\mu(x) = -\frac{1}{2}B_2(\{x-1/2\}) = -\frac{1}{2}|x-1/2|^2 + \frac{1}{2}|x-1/2| - \frac{1}{12}, \quad \beta = 1, \text{ and } M = \frac{13}{12}.$$

Then by Lemma 2 in the Supplementary Material and some calculations similar to those in Example 1, we have

$$\mu_1 = -\frac{1}{48s}+\frac{(-1)^s}{16s}, \quad \mu_2 = \frac{7s^3}{720}-\frac{s}{72}-\frac{13}{480s}-\frac{(-1)^s}{32s},$$
$$\mu_3 = \frac{7s^3}{2880}-\frac{5s}{576}+\frac{s(-1)^s}{64}-\frac{1}{640s}-\frac{15(-1)^s}{640s}, \text{ and}$$
$$\Phi_{\mathrm{CD}}(D) = \frac{g_{\mathrm{CD}}(D)}{4n^2m(m-1)s^2} + \tilde{C}_{\mathrm{CD}}(m,s),$$

where $g_{\mathrm{CD}}(D) = g_{\mathrm{GD}}(D)$ in (13) and

$$\tilde{C}_{\mathrm{CD}}(m,s) = \left(\frac{1}{36}+\frac{1}{8s^2}+\frac{7}{192s^4}+\frac{(-1)^s}{64s^4}\right) + \frac{1}{m-1}\left(\frac{1}{60}-\frac{1}{12s^2}+\frac{1}{15s^4}\right).$$

One can verify that this coincides with Theorem 2 of Sun, Wang & Xu (2019). Thus Theorem 2 generalizes the result in Sun, Wang & Xu (2019).

Example 3 (The SD)**.** For an (n, s^m) design $D = (x_{ik})$

$$\mathrm{SD}(D) = \left(\frac{4}{3}\right)^m - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(1 + 2\left(\frac{2x_{ik}+1}{2s}\right) - 2\left(\frac{2x_{ik}+1}{2s}\right)^2\right) + \frac{2^m}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(1 - \left|\frac{x_{ik}-x_{jk}}{s}\right|\right).$$

Following Hickernell (1998a), the SD is a special case of the GD with

$$\mu(x) = -\frac{1}{2}B_2(x) = -\frac{1}{2}\left(x - \frac{1}{2}\right)^2 + \frac{1}{24}, \quad \beta = 2, \text{ and } M = \frac{4}{3}.$$

Similar to Examples 1 and 2, we have

$$\mu_1 = \frac{1}{24s}, \quad \mu_2 = -\frac{s^3}{90} + \frac{5s}{72} - \frac{7}{120s}, \quad \mu_3 = -\frac{s^3}{360} + \frac{s}{36} - \frac{1}{40s}, \text{ and}$$

$$\Phi_{\mathrm{SD}}(D) = \frac{4g_{\mathrm{SD}}(D)}{n^2m(m-1)s^2} + \tilde{C}_{\mathrm{SD}}(m,s),$$

where $g_{\mathrm{SD}}(D) = g_{\mathrm{GD}}(D)$ in (13) and

$$\tilde{C}_{\mathrm{SD}}(m,s) = \left(\frac{4}{9} + \frac{5}{6s^4}\right) + \frac{1}{m-1}\left(\frac{4}{15} - \frac{4}{3s^2} + \frac{16}{15s^4}\right).$$

We summarize Examples 1–3 in the following corollary.

Corollary 1. *For an (n, s^m) design $D = (x_{ik})$, the uniform projection criteria under the (modified) L_2-star discrepancy, the CD, and the SD are all equivalent to minimizing $g_{\mathrm{GD}}(D)$, as defined in (13).*

Now we consider the lower and upper bounds for the uniform projection criterion Φ_{GD}. As all two-dimensional projection GD's are equivalent by Theorem 2, in the following we only consider lower and upper bounds for

$$g_{\mathrm{GD}}(D) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_1^2(x_i, x_j) - \frac{2}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{n} d_1(x_i, x_j)\right)^2,$$

defined in (13), which is a quadratic form of $\{d_1(x_i, x_j), i < j\}$ and has been studied for the CD in Theorem 3 of Sun, Wang & Xu (2019) and Lemma 5 of Wang, Sun & Xu (2020). We summarize and rephrase these results in the following theorem in terms of g_{GD}.

Theorem 3. *For a U-type (n, s^m) design D, we have $g_{\mathrm{GD}}^{LB} \leq g_{\mathrm{GD}}(D) \leq g_{\mathrm{GD}}^{UB}$, where*

$$g_{\mathrm{GD}}^{LB} = -\frac{(n-2)n^2m^2\left(s^2-1\right)^2}{9(n-1)s^2} \quad \text{and} \quad g_{\mathrm{GD}}^{UB} = -\frac{n^2m^2\left(s^4 - 5s^2 + 4\right)}{18s^2}.$$

Furthermore, the lower bound g_{GD}^{LB} is achieved if and only if $d_1(x_i, x_j) = \overline{d}_1$ in (11) for all $1 \leq i < j \leq n$.

Remark 1. Using Theorem 4 of Sun, Wang & Xu (2019), we can get another lower bound of $g_{\mathrm{GD}}(D)$ for U-type (n, s^m) designs, that is

$$g_{\mathrm{GD}}(D) \geq g_{\mathrm{GD}}^{LB'} = -\frac{n^2 m\left(s^2-1\right)\left[(5m-2)s^2-5m-7\right]}{45s^2},$$

and this bound is achieved if and only if D is an $OA(n, s^m, 2)$. The obtaining of the lower bound $g_{\mathrm{GD}}^{LB'}$ utilizes the lower bounds for the CD in Ma, Fang & Lin (2003). Therefore, we have that $g_{\mathrm{GD}}(D) \geq \max\left\{g_{\mathrm{GD}}^{LB}, g_{\mathrm{GD}}^{LB'}\right\}$. The lower bound $g_{\mathrm{GD}}^{LB'}$ is sharper when $m \leq (2s^2+7)(n-1)/(5s^2-5)$, and g_{GD}^{LB} is sharper otherwise (Wang, Sun & Xu, 2020). In this article, we are more interested in g_{GD}^{LB}, as it is more related to the maximin L_1-distance criterion, as g_{GD}^{LB} is attained if and only if the design D is an L_1-equidistant maximin distance U-type design. Thus, in the following we focus only on the lower bound g_{GD}^{LB}.

Lower and upper bounds for the uniform projection criterion Φ_{GD}, say Φ_{GD}^{LB}, $\Phi_{\mathrm{GD}}^{LB'}$, and Φ_{GD}^{UB} (corresponding to g_{GD}^{LB}, $g_{\mathrm{GD}}^{LB'}$, and g_{GD}^{UB}, respectively), based on any explicit GD can be easily obtained by (12), Theorem 3, and Remark 1. In particular

- for the (modified) L_2-star discrepancy

$$\Phi_{\mathrm{D}_2^*}^{LB} = \frac{5m\left(n\left(64s^2+7\right)+8s^4-80s^2+1\right)-(n-1)\left(16s^4+360s^2-21\right)}{1440(m-1)(n-1)s^4},$$

$$\Phi_{\mathrm{D}_2^*}^{LB'} = \frac{64s^2+7}{288s^4}, \quad \Phi_{\mathrm{D}_2^*}^{UB} = \frac{5m\left(4s^4+68s^2-1\right)-16s^4-360s^2+21}{1440(m-1)s^4};$$

- for the CD

$$\Phi_{\mathrm{CD}}^{LB} = \frac{5m(4s^4+2(13n-17)s^2-n+5)-(n-1)(8s^4+150s^2-33)}{720(n-1)(m-1)s^4} + \frac{1+(-1)^s}{64s^4},$$

$$\Phi_{\mathrm{CD}}^{LB'} = \frac{26s^2-1}{144s^4} + \frac{1+(-1)^s}{64s^4},$$

$$\Phi_{\mathrm{CD}}^{UB} = \frac{(10m-8)s^4+(140m-150)s^2-25m+33}{720(m-1)s^4} + \frac{(-1)^s+1}{64s^4}; \textit{and}$$

- for the SD

$$\Phi_{\mathrm{SD}}^{LB} = \frac{5m\left(16(n-2)s^2+7n+8s^4+1\right)-(n-1)\left(16s^4+120s^2-21\right)}{90(m-1)(n-1)s^4},$$

$$\Phi_{\mathrm{SD}}^{LB'} = \frac{7}{18s^4} + \frac{8}{9s^2}, \quad \Phi_{\mathrm{SD}}^{UB} = \frac{5m\left(4s^4+20s^2-1\right)-16s^4-120s^2+21}{90(m-1)s^4}.$$

We can evaluate the quality of a design D by the relative efficiency

$$\Phi_{\mathrm{GD}}^{RE} = \frac{\Phi_{\mathrm{GD}}^{UB}-\Phi_{\mathrm{GD}}(D)}{\Phi_{\mathrm{GD}}^{UB}-\Phi_{\mathrm{GD}}^{LB}} = \frac{g_{\mathrm{GD}}^{UB}-g_{\mathrm{GD}}(D)}{g_{\mathrm{GD}}^{UB}-g_{\mathrm{GD}}^{LB}}.$$

Here, only the value and bounds of $g_{\text{GD}}(D)$ are required in the calculation. Designs with higher Φ_{GD}^{RE} are preferred as space-filling designs with better two-dimensional projection uniformity; in particular, $\Phi_{\text{GD}}^{RE} = 1$ for a maximin L_1-equidistant design, whereas Φ_{GD}^{RE} can be small for a bad design. For example, if we take $s = n$ in (S5) in the Supplementary Material to get an LHD $\tilde{D}$, then $\Phi_{\text{GD}}^{RE}(\tilde{D}) = 1/5 + 2/(5n) \to 1/5$ as $n \to \infty$.

3.2. Wrap-around L_2-discrepancy and Mixture Discrepancy

In this subsection, we focus on the projection uniformity under the WD proposed by Hickernell (1998b) and the MD proposed by Zhou, Fang & Ning (2013). For an (n, s^m) design $D = (x_{ik})$,

$$\text{WD}(D) = -\left(\frac{4}{3}\right)^m + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(\frac{3}{2} - \left|\frac{x_{ik} - x_{jk}}{s}\right| + \left|\frac{x_{ik} - x_{jk}}{s}\right|^2\right)$$

and

$$\begin{aligned}\text{MD}(D) = &\left(\frac{19}{12}\right)^m - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(\frac{5}{3} - \frac{1}{4}\left|\frac{2x_{ik} - s + 1}{2s}\right| - \frac{1}{4}\left|\frac{2x_{ik} - s + 1}{2s}\right|^2\right)\\ &+ \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(\frac{15}{8} - \frac{1}{4}\left|\frac{2x_{ik} - s + 1}{2s}\right| - \frac{1}{4}\left|\frac{2x_{jk} - s + 1}{2s}\right|\right.\\ &\left. - \frac{3}{4}\left|\frac{x_{ik} - x_{jk}}{s}\right| + \frac{1}{2}\left|\frac{x_{ik} - x_{jk}}{s}\right|^2\right).\end{aligned}$$

They can be induced by taking $f(x, y) = 3/2 - |x - y| + |x - y|^2$ and

$$f(x, y) = \frac{15}{8} - \frac{1}{4}\left|x - \frac{1}{2}\right| - \frac{1}{4}\left|y - \frac{1}{2}\right| - \frac{3}{4}|x - y| + \frac{1}{2}|x - y|^2$$

as the kernel functions in (1).

Theorem 4. *For a U-type (n, s^m) design $D = (x_{ik})$,*

$$\Phi_{\text{WD}}(D) = \frac{g_{\text{WD}}(D)}{n^2 m(m-1)s^4} + \tilde{C}_{\text{WD}}(m, s), \tag{14}$$

where

$$g_{\text{WD}}(D) = \sum_{i=1}^{n}\sum_{j=1}^{n}\left(s \cdot d_1(x_i, x_j) - d_2(x_i, x_j)\right)^2, \tag{15}$$

$d_p(x_i, x_j)$ is defined in (10) with $p = 1, 2$, and

$$\tilde{C}_{\text{WD}}(m, s) = -\frac{1}{36} - \frac{1}{30(m-1)} + \frac{1}{2s^2} + \frac{1}{30(m-1)s^4}.$$

The proofs of Theorem 4 and all subsequent theorems are given in the Supplementary Material. Theorem 4 is parallel to Theorem 2; it shows that the uniform projection criterion under the WD is only related to $s \cdot d_1(x_i, x_j) - d_2(x_i, x_j)$, that is, a combination of L_1- and L_2-distances, for a U-type design $D = (x_{ij})$. By the fact that for any two rows x_i and x_j,

$$d_2(x_i, x_j) = \sum_{k=1}^{m} (x_{ik} - x_{jk})^2 \leq (s-1) \sum_{k=1}^{m} |x_{ik} - x_{jk}| = (s-1) d_1(x_i, x_j), \tag{16}$$

we always have $s \cdot d_1(x_i, x_j) - d_2(x_i, x_j) \geq 0$.

The following theorem considers the lower and upper bounds for the $g_{\mathrm{WD}}(D)$ defined in (15).

Theorem 5. *For a U-type (n, s^m) design D, we have $g_{\mathrm{WD}}^{LB} \leq g_{\mathrm{WD}}(D) \leq g_{\mathrm{WD}}^{UB}$, where*

$$g_{\mathrm{WD}}^{LB} = \frac{m^2 n^3 \left(s^2 - 1\right)^2}{36(n-1)} \quad \text{and} \quad g_{\mathrm{WD}}^{UB} = \frac{n^2 m^2 \left(s^4 - 1\right)}{30}.$$

Furthermore, the lower bound g_{WD}^{LB} is achieved if and only if $s \cdot d_1(x_i, x_j) - d_2(x_i, x_j) = nm(s^2 - 1)/(6n - 6)$ for all $1 \leq i < j \leq n$, and the upper bound g_{WD}^{UB} is achieved when D is equal to the design $\tilde{D}$ in (S5) in the Supplementary Material.

For the MD, Theorem 6 gives a conclusion similar to that of Theorem 4.

Theorem 6. *For a U-type (n, s^m) design $D = (x_{ik})$,*

$$\Phi_{\mathrm{MD}}(D) = \frac{g_{\mathrm{MD}}(D)}{16 n^2 m (m-1) s^4} + \tilde{C}_{\mathrm{MD}}(m, s), \tag{17}$$

where

$$g_{\mathrm{MD}}(D) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(3s \cdot d_1(x_i, x_j) - 2 d_2(x_i, x_j)\right)^2 - \frac{2}{n} \sum_{i=1}^{n} \left[\sum_{j=1}^{n} (3s \cdot d_1(x_i, x_j) - 2 d_2(x_i, x_j)) \right]^2, \tag{18}$$

$d_p(x_i, x_j)$ is defined in (10) with $p = 1, 2$ and

$$\tilde{C}_{\mathrm{MD}}(m, s) = \frac{1}{36} + \frac{49}{144 s^2} + \frac{59}{768 s^4} - \frac{17(-1)^s}{768 s^4} + \frac{1}{48(m-1)} \left(1 - \frac{5}{s^2} + \frac{4}{s^4}\right).$$

For $g_{\mathrm{MD}}(D)$ defined in (18), it also follows by (16) that $3s \cdot d_1(x_i, x_j) - 2 d_2(x_i, x_j) \geq 0$. Bounds for $g_{\mathrm{MD}}(D)$ are given in Theorem 7.

Theorem 7. *For a U-type (n, s^m) design D, we have $g_{\mathrm{MD}}^{LB} \leq g_{\mathrm{MD}}(D) \leq g_{\mathrm{MD}}^{UB}$, where*

$$g_{\mathrm{MD}}^{LB} = -\frac{4 m^2 (n-2) n^2 \left(s^2 - 1\right)^2}{9(n-1)} \quad \text{and} \quad g_{\mathrm{MD}}^{UB} = -\frac{29 m^2 n^2 \left(s^4 - 5 s^2 + 4\right)}{90}.$$

Furthermore, the lower bound g_{WD}^{LB} is achieved if and only if $3s \cdot d_1(x_i, x_j) - 2 d_2(x_i, x_j) = 2mn(s^2 - 1)/(3n - 3)$ for all $1 \leq i < j \leq n$.

When D is simultaneously an L_1- and L_2-equidistant maximin distance U-type design, the conditions that $s \cdot d_1(x_i, x_j) - d_2(x_i, x_j) = nm(s^2-1)/(6n-6)$ and $3s \cdot d_1(x_i, x_j) - 2d_2(x_i, x_j) = 2mn(s^2-1)/(3n-3)$ for all $1 \le i < j \le n$ are satisfied, and thus the lower bounds g_{WD}^{LB} and g_{MD}^{LB} are both attained. By Theorems 4–7, we can get lower and upper bounds for Φ_{WD} and Φ_{MD} as

$$\Phi_{\mathrm{WD}}^{LB} = \frac{(5m-n+1)s^4 + 10[m(8n-9) - 9n + 9]s^2 + 5mn + 6n - 6}{180(m-1)(n-1)s^4},$$

$$\Phi_{\mathrm{WD}}^{UB} = \frac{s^4 + 90s^2 - 6}{180s^4},$$

$$\Phi_{\mathrm{MD}}^{LB} = \frac{m\left[16(57n-65)s^2 + 113n + 64s^4 - 49\right] - (n-1)\left[16s^2\left(s^2+64\right) - 15\right]}{2304(m-1)(n-1)s^4} - \frac{17(-1)^s}{768s^4},$$

$$\Phi_{\mathrm{MD}}^{UB} = \frac{m\left(88s^4 + 5080s^2 - 43\right) - 80\left(s^2+64\right)s^2 + 75}{11520(m-1)s^4} - \frac{17(-1)^s}{768s^4},$$

and define the relative efficiencies Φ_{WD}^{RE} and Φ_{MD}^{RE} similarly to how we defined Φ_{GD}^{RE} for evaluating any U-type design D.

At the end of this section, we mention that all the formulas for the GD, WD, and MD in Theorems 2, 4, and 6 are also important from the computational perspective. Computing discrepancy with (12), (14), or (17) has a complexity of $O(n^2m)$, which is faster than computing it with (3), which has a complexity of $O(n^2m^2)$. The complexity $O(n^2m)$ is the same order of complexity as computing the popular Maxmin criterion (Morris & Mitchell, 1995) and MaxPro criterion (Joseph, Gul & Ba, 2015). As an application, standard stochastic searching algorithms such as simulated annealing or threshold-accepting algorithms can be used for constructing uniform projection U-type designs based on the proposed Φ_{GD}, Φ_{WD}, and Φ_{MD} criteria. We give the details of such a threshold-accepting algorithm in Section 3.1 of the Supplementary Material.

4. SPACE-FILLING DESIGNS WITH GOOD PROJECTION UNIFORMITY

In this section, we investigate the two-dimensional projection uniformity of several families of space-filling designs. These designs were proposed using the maximin distance criterion without taking projection properties into account, as well as other optimal projection criteria from different perspectives. Using the projection uniformity theories and the numerical simulations, we show that these designs also have good two-dimensional projection uniformity and thus are suitable for factor screening in computer experiments (Moon, Dean & Santner, 2012; Woods & Lewis, 2016).

4.1. Latin Hypercube Designs Based on Good Lattice Point Designs

LHDs based on good lattice point (GLP) designs have been recently studied by Wang, Xiao & Xu (2018), and Zhou & Xu (2015) under the maximin L_1-distance criterion, and by Sun, Wang & Xu (2019), and Wang, Sun & Xu (2020) under the uniform projection Φ_{CD} criterion. Let $(h_1, \ldots, h_m)$ be a row vector with all elements coprime to n, where n is a positive integer. A GLP design is an $LHD(n, m)$, denoted as $D = (x_{ik})$, constructed by $x_{ik} = i \times h_k \ (mod\ n)$ for $i = 1, \ldots, n$ and $k = 1, \ldots, m$. Obviously, for a given n, GLP designs exist for any $1 \le m \le \varphi(n)$, where $\varphi(n)$ is the number of positive integers coprime to n and less than n. Let

$$W(x) = \begin{cases} 2x, & 0 \le x < n/2 \\ 2(n-x)-1, & n/2 \le x < n, \end{cases} \quad \text{and} \quad w(x) = \begin{cases} 2x, & 0 \le x < n/2 \\ 2(n-x), & n/2 \le x < n. \end{cases}$$

We consider the following three families of LHDs based on GLP designs.

- $LHD(n, n)$ where $n = (p - 1)/2$ and p is an odd prime.

Let D be a $(2n + 1) \times (2n)$ GLP design and A_1 be the $n \times n$ leading principal submatrix of D, where $n = (p - 1)/2$ and p is an odd prime. Theorem 4 of Wang, Xiao & Xu (2018) shows that $E = w(A_1)/2$ is an L_1-equidistant $LHD(n, n)$ with $d_1(E) = \overline{d}_1 = n(n + 1)/3$, where $w(A_1)$ represents the $n \times n$ design with all entries in A_1 transformed by $w(\cdot)$. By Theorem 3, $g_{\mathrm{GD}}(E)$ is equal to g^{LB}_{GD} defined in Theorem 3, and the relative efficiency $\Phi^{RE}_{\mathrm{GD}}(E)$ (including $\Phi^{RE}_{\mathrm{D}^*_2}$, Φ^{RE}_{CD}, and Φ^{RE}_{SD}) is always 1.

It is known that two rows with a larger L_1-distance between them also tend to have larger L_2-distance between them, and vice versa. Therefore, the above L_1-equidistant E should also be efficient under the maximin L_2-distance criterion. We expect that E also has good performance under the Φ_{WD} and Φ_{MD} criteria. To examine this, we plot in Figure 1 the Φ^{RE}_{GD} (solid line), Φ^{RE}_{WD} (dashed line), and Φ^{RE}_{MD} (dotted line) values for the $LHD(n, n)$'s $E = (x_{ik})$ with $p < 100$ (see the subplot of $n = (p - 1)/2$). We see that the relative Φ_{WD}- and Φ_{MD}-efficiencies are also very close to 1 (the Φ^{RE}_{GD} line) and approach 1 quickly as p increases.

- $LHD(n, n - 1)$ where $n = p$ is an odd prime.

Let D be an $n \times (n - 1)$ GLP design, where $n = p$ is an odd prime. For $b \in \mathcal{Z}_n = \{0, \ldots, n - 1\}$, let $D_b = D + b = (x_{ik} + b) \pmod n$ be a linear permutation of the GLP design D. Let $E_{b^*} = W(D_{b^*})$, where $b^* = W^{-1}\left((n - 1)/2 \pm c\right)$,

$$c = \begin{cases} c_0, & c_0 \geq \sqrt{(n^2 - 4)/12} - 1/2, \\ c_0 + 1, & c_0 < \sqrt{(n^2 - 4)/12} - 1/2, \end{cases}$$

and $c_0 = \lfloor \sqrt{(n^2 - 1)/12} \rfloor$. Theorem 4 of Sun, Wang & Xu (2019) and Proposition 3 of Wang, Sun & Xu (2020) show that the LHD E_{b^*} not only has a large minimum L_1-distance (it nearly

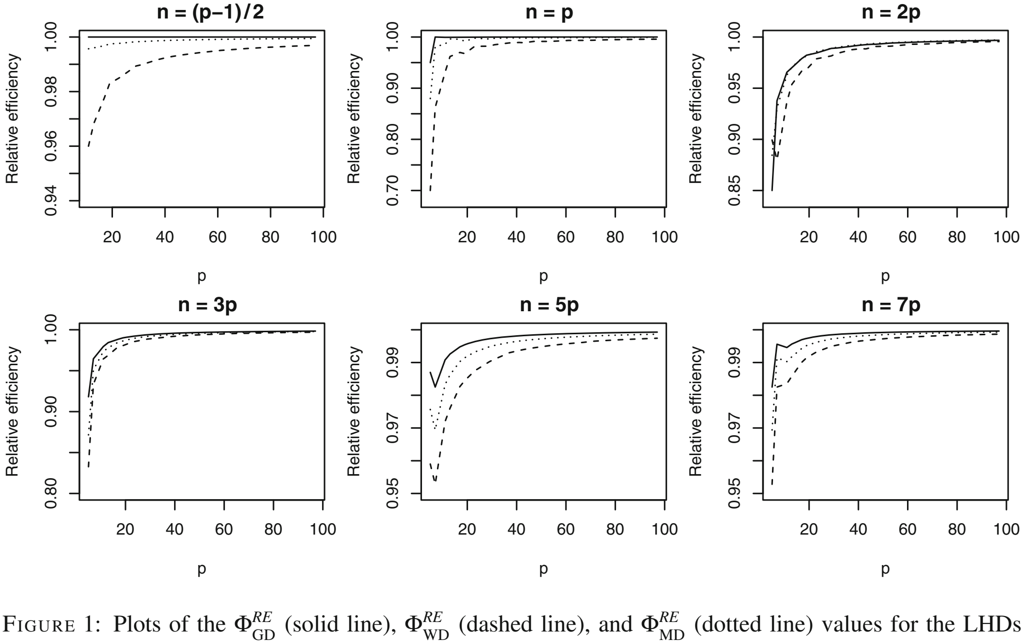

FIGURE 1: Plots of the Φ^{RE}_{GD} (solid line), Φ^{RE}_{WD} (dashed line), and Φ^{RE}_{MD} (dotted line) values for the LHDs with $n = (p - 1)/2, p, 2p, 3p, 5p, 7p, p < 100$.

achieves the bound in Lemma 1) but also minimizes $\Phi_{\mathrm{CD}}(E_b)$ among all $b \in \mathcal{Z}_n$ with its value smaller than $(1+5/n^2)\Phi_{\mathrm{CD}}^{LB}$. Since all the GDs are equivalent by our Theorem 2, we have that $\Phi_{\mathrm{GD}}^{RE}(E_{b^*}) = \Phi_{\mathrm{D}_2^*}^{RE}(E_{b^*}) = \Phi_{\mathrm{SD}}^{RE}(E_{b^*}) = \Phi_{\mathrm{CD}}^{RE}(E_{b^*}) = 1 - O(1/n^3)$. We also expect that E_{b^*} performs well under the Φ_{WD} and Φ_{MD} criteria. Figure 1 shows the plots of the Φ_{GD}^{RE}, Φ_{WD}^{RE}, and Φ_{MD}^{RE} values for the $LHD(n, n-1)$'s E_{b^*} with $p < 100$ (see the subplot of $n = p$). All three of the relative uniform projection efficiencies are higher than 0.9 when $p > 7$ and approach 1 quickly as p increases.

- $LHD(n, (k-1)(p-1))$ where $n = kp$, $k \neq p$, k is a prime, and p is an odd prime.

Let D be an $n \times (k-1)(p-1)$ GLP design, $D_b = D + b = (x_{ik} + b) \pmod n$ where $n = kp$, k is a prime and p is an odd prime, and $b = \lfloor n(1 + 1/\sqrt{3})/4 \rfloor$. Then $E_b = W(D_b)$ gives a good space-filling $LHD(n, (k-1)(p-1))$. We consider the cases of $k = 2, 3, 5$, and 7 for illustration. By Wang, Xiao & Xu (2018), the LHD E_b has large minimum L_1-distance. By Wang, Sun & Xu (2020) and our Theorem 2, the relative efficiency $\Phi_{\mathrm{GD}}^{RE}(E_b) = \Phi_{\mathrm{D}_2^*}^{RE}(E_b) = \Phi_{\mathrm{CD}}^{RE}(E_b) = \Phi_{\mathrm{SD}}^{RE}(E_b)$ is very high and approaches 1 quickly as p grows. The subplots titled with $n = kp$ ($k = 2, 3, 5, 7$) of Figure 1 show the relative efficiencies of E_b $\left(\Phi_{\mathrm{GD}}^{RE}, \Phi_{\mathrm{WD}}^{RE}, \text{and } \Phi_{\mathrm{MD}}^{RE}\right)$ for $p < 100$. As expected, the $LHD(n, (k-1)(p-1))$'s E_b are also very efficient under the Φ_{WD} and Φ_{MD} criteria.

4.2. Maximin Distance U-type (n, s^m) Designs with $s < n$

Suppose that A is a U-type (n, s^{m_1}) design and B is a U-type (s, q^{m_2}) design. The replacement method generates a U-type $(n, q^{m_1 m_2})$ design by replacing the uth level of A by the $(u+1)$th row of B for $u = 0, 1, \ldots, s-1$. Using B as the maximin or nearly maximin distance LHDs such as those constructed in Wang, Xiao & Xu (2018), Li, Liu & Tang (2021) obtained many maximin or nearly maximin distance U-type designs. These designs are also expected to be highly efficient under the uniform projection Φ_{GD}, Φ_{WD}, and Φ_{MD} criteria. For illustration, we generate the designs in Tables 1 and 2 of Li, Liu & Tang (2021) (by their Theorem 2 and Propositions 1 and 2) with run size $n < 100$ and calculate their relative efficiencies Φ_{GD}^{RE}, Φ_{WD}^{RE}, and Φ_{MD}^{RE}. The numerical results are shown in Table 1, in which we can see that all these U-type designs have relative efficiencies larger than 0.99 under the three uniform projection criteria.

4.3. MaxPro Designs and Minimax Projection Designs

We also explore the two-dimensional projection uniformity of three types of popular space-filling designs constructed to have good projections, namely MaxPro designs (Joseph, Gul & Ba, 2015), minimax designs and minimax projection designs by Mak & Joseph (2018). Let $D = (x_{ij})$ be an

TABLE 1: Relative efficiency values Φ_{GD}^{RE}, Φ_{WD}^{RE}, and Φ_{MD}^{RE} for some space-filling U-type (n, s^m) designs.

(n, s^m)	Φ_{GD}^{RE}	Φ_{WD}^{RE}	Φ_{MD}^{RE}	(n, s^m)	Φ_{GD}^{RE}	Φ_{WD}^{RE}	Φ_{MD}^{RE}
$(9, 3^{12})$	1	1	1	$(25, 5^{30})$	0.9950	0.9903	0.9928
$(27, 3^{39})$	1	1	1	$(49, 7^{48})$	1	0.9937	0.9988
$(81, 3^{120})$	1	1	1	$(64, 8^{72})$	1	0.9989	0.9998
$(16, 4^{15})$	0.9900	1	0.9962	$(81, 9^{80})$	0.9983	0.9995	0.9992
$(64, 4^{63})$	0.9978	1	0.9992	$(81, 9^{90})$	1	0.9992	0.9998
$(25, 5^{24})$	1	0.9987	0.9997				

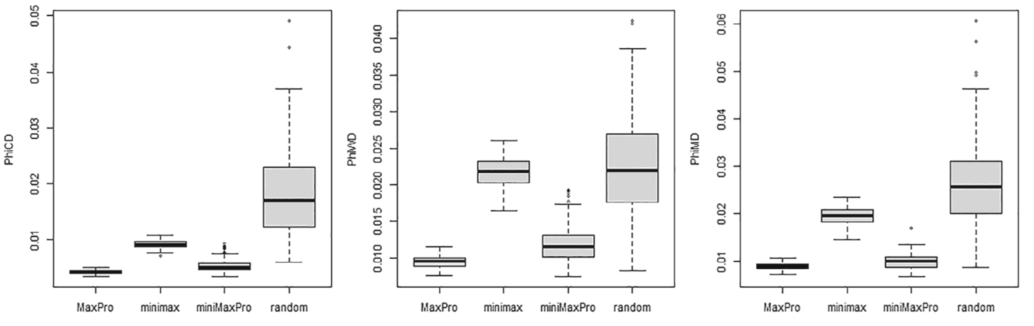

FIGURE 2: Box plots of the $\Phi_{\rm CD}$, $\Phi_{\rm WD}$, and $\Phi_{\rm MD}$ values of the 100 MaxPro, minimax, minimax projection, and random designs.

$n \times m$ design with $x_{ij} \in [0, 1]$ (not necessarily an LHD or a U-type design). The MaxPro criterion is to minimize

$$\psi(D) = \left\{ \frac{1}{\binom{n}{2}} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{\prod_{k=1}^{m} (x_{ik} - x_{jk})^2} \right\}^{1/m}.$$

A minimax design minimizes the maximum distance from any point in this space to its nearest design point. A minimax projection design is obtained by refining a minimax design using the MaxPro criterion ψ.

The R packages `MaxPro` and `minimaxdesign` developed by Joseph, Gul & Ba (2015) and by Mak & Joseph (2018), respectively, are efficient for generating the three types of designs. We numerically study the performances of the three types of designs using nine simulation settings with $n = 15, 20, 30$ and $m = 3, 5, 8$. For each (n, m) combination, we run the `MaxPro`, `minimax`, and `miniMaxPro` functions 100 times with default settings to generate 100 MaxPro, minimax, and minimax projection designs and then compute their $\Phi_{\rm CD}$, $\Phi_{\rm WD}$, and $\Phi_{\rm MD}$ values. The performances under the (modified) L_2-star discrepancy and the SD are close to those under the CD and thus are omitted. Note that the computation of $\Phi_{\rm Disc}$ under a given L_2-type discrepancy should use the original definition (3) since these designs are not U-type designs. Figure 2 shows the box plots of the $\Phi_{\rm CD}$, $\Phi_{\rm WD}$, and $\Phi_{\rm MD}$ values of different designs for the case of $(n = 20, m = 3)$. The results for the other eight cases are similar. The plots of 100 random designs uniformly distributed over the design space are also provided for comparison. From Figure 2, we see that the MaxPro and minimax projection designs have much better projection uniformity than the minimax designs and random designs under the $\Phi_{\rm CD}$, $\Phi_{\rm WD}$, and $\Phi_{\rm MD}$ criteria. This meets our expectations because the MaxPro and minimax projection criteria all focus on projection properties. The MaxPro designs slightly outperform the minimax projection designs. The minimax designs are better than the random designs under the $\Phi_{\rm CD}$ and $\Phi_{\rm MD}$ criteria. Notice that the R package `MaxPro` can also generate MaxPro LHDs. When restricted to LHDs, the MaxPro LHDs again have good projection uniformity; see the numerical comparisons in Section 3.2 of the Supplementary Material for more information.

5. DISCUSSION

A uniform projection criterion that focuses on two-dimensional uniformity is appealing for space-filling designs. We established a general formula of two-dimensional uniformity for U-type designs and further applied it to obtain more explicit results for the commonly used discrepancies. These results generalized and improved the existing results and also revealed new connections between the two popular space-filling criteria—uniformity and the maximin distance. We also studied several recently proposed families of optimal space-filling designs. These designs were shown to have desirable performance under various uniform projection criteria. Therefore, these designs are well adapted for computer experiments, especially for early stage experiments where there are a large number of factors to be explored but only a few of them are important.

It should be mentioned that the criterion function (3) takes the average discrepancy over all two-dimensional projections. Alternatively, one can define a criterion to minimize $\max_{|u|=2} \mathrm{Disc}(D_u, K)$, that is, the worst case discrepancy value over all possible two-dimensional projections in D. Although the two criteria are not equivalent, our preliminary numerical studies show that minimizing (3) tends to produce a design with a small $\max_{|u|=2} \mathrm{Disc}(D_u, K)$ value; see Section 3.3 of the Supplementary Material for more information.

Some possible future studies are presented. First, this article focuses on symmetric designs (i.e., where the levels of all factors are equal). In practice, asymmetric designs (i.e., designs with at least two different levels) are also frequently demanded; see Elsawah & Qin (2016) and Yang, Zhou & Zhang (2019) for some recent developments. A natural progression of this work is to extend the obtained results to asymmetric designs. Second, it will be meaningful to construct uniform projection U-type designs by combining the obtained results with some combinatorial methods. A possible method with great theoretical beauty is rotating groups of factors of orthogonal arrays (Sun, Pang & Liu, 2011; Sun & Tang, 2017). Finally, it is an interesting and important problem to relate the uniform projection criterion (3) to other statistical design criteria. Recently, Sun & Tang (2021) showed that the uniform projection criterion is strongly related to the stratification properties of the design. They established novel connections between the uniform projection criterion and strong orthogonal arrays. Under the Gaussian process model, Joseph, Gul & Ba (2015) showed that the MaxPro criterion tends to agree with the maximum entropy criterion. In Section 3.4 of the Supplementary Material, we provide a preliminary study on the connection between the uniform projection criterion and the maximum entropy criterion. Our numerical results suggest that the uniform projection criterion also tends to agree with the maximum entropy criterion. We will explore more rigorous theoretical justifications of the uniform projection criterion along the lines of Sun & Tang (2021) and Joseph, Gul & Ba (2015) in the future.

ACKNOWLEDGEMENTS

The authors sincerely thank the editor, the associate editor, and the two referees for their comments, which have led to the improvement of the paper. Sixu Liu and Yaping Wang are co-first authors. Yaping Wang was supported by NSFC Grant Nos. 11901199, 11971171, Shanghai Chenguang Program Grant No. 19CG26, and the KLAS Research Fund Grant No. 130028906 of Northeast Normal University. Fasheng Sun was supported by the NSFC Grant No. 11971098 and the National Key Research and Development Program of China (No. 2020YFA0714102).

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Received 4 March 2021
Accepted 17 November 2021