Statistica Sinica Preprint No: SS-2025-0279	
Title	Space-filling Designs with Kronecker Product Structures under Kernel-Based Criteria
Manuscript ID	SS-2025-0279
URL	http://www.stat.sinica.edu.tw/statistica/
DOI	10.5705/ss.202025.0279
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Notice: Accepted author version.	

SPACE-FILLING DESIGNS WITH KRONECKER PRODUCT STRUCTURES UNDER KERNEL-BASED CRITERIA

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Abstract: Computer experiments have been widely used in various fields. Among different design types, space-filling designs stand out as the most common choice for computer experiments due to their effectiveness in thoroughly exploring the experimental region. Extensive research has been conducted on the space-filling criteria. However, there are relatively few studies developing a systematic framework for relationships among most space-filling criteria. Kernel functions possess numerous elegant properties, and some space-filling criteria also have inherent connections with them. This paper establishes links among different space-filling criteria via their expressions in the form of kernel functions. Focusing on the designs with Kronecker product structure, this paper provides explicit expressions and associated theoretical results for kernel-based space-filling criteria. In addition, construction methods for optimal designs with Kronecker product structure are also proposed. Moreover, an algorithm is proposed to generate a series of space-filling designs that have better performance compared with other designs.

Key words and phrases: Discrepancy; Kernel function; Maximin distance; Uniform design

1. Introduction

In the past decades, computer experiments have been widely used in industry,

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aerospace and so on due to their high efficiencies. However, the code of a computer experiment is usually so complex that each implementation may take a lot of time. Thus, a few representative data points should be selected to fit a model for the computer experiment. Space-filling design whose data points fill the design region as much as possible is a good choice. The key problems are how to evaluate the space-filling property of a design and construct designs based on some given criteria.

To evaluate the space-filling property of a design, various commonly used criteria have been proposed, such as distance-based criteria, discrepancies, and projection-based criterion. For distance-based criteria, the maximin distance criterion proposed by Johnson, Moore and Ylvisaker (1990) is widely adopted. Zhou and Xu (2014) extended this criterion to select the one with the least number of pairs achieving the minimum distance among designs that maximize the minimum distance. Designs that perform well under discrepancies are referred to as uniform designs, which contain fruitful results in both theory and application. One can refer to Fang et al. (2018) for various discrepancies. In addition, Joseph, Gul and Ba (2015) proposed the maximum projection criterion from the perspective of Gaussian correlation function.

For constructing space-filling designs, there are mainly two classes of methods. One class is deterministic methods, see e.g. Zhou and Xu (2015); Wang, Xiao and Xu (2018); Li, Liu and Tang (2021); Li, Tian and Liu (2024) and references therein. The other class is algorithmic optimization methods. For example, Zhou and Fang (2013) proposed a mixture method to construct uniform designs with large sizes by improving the threshold accepting (TA) algorithm. Among various construction methods, the

Kronecker product is a powerful tool and has been widely used to construct various space-filling designs, such as orthogonal and nearly orthogonal designs (Bingham, Sitter and Tang, 2009), orthogonal Latin hypercube designs (Lin et al., 2010), and orthogonal arrays with high strength (Pang et al., 2021).

Existing studies on the relationships among space-filling criteria often focus on pairs of criteria. For example, Wang, Sun and Xu (2022) investigated the connection between column-orthogonality and L_2-distance, as well as that between projection uniformity and maximin L_1-distance. However, a systematic framework for investigating the relationships among most space-filling criteria remains lacking. In fact, some space-filling criteria have inherent connections with kernel functions, for example, discrepancies are derived based on reproducing kernels, and the maximum projection criterion is derived from Gaussian kernels. Kernel functions have been extensively studied and possess numerous favorable properties (Van Den Berg, Christensen and Ressel, 2012), which can provide new perspectives and tools to derive novel results related to space-filling criteria. We prove that most space-filling criteria can be expressed in the form of kernel functions, which are referred to as kernel-based space-filling criteria. For a design with Kronecker product structure, we provide a specific expression and corresponding theoretical results under the kernel-based space-filling criterion. Under this criterion, we provide corresponding optimal designs. Furthermore, under the maximin L_2-distance criterion, as a specific space-filling criterion, we provide an additional method for constructing optimal designs with Kronecker product structure. For some experimental cases, it is unnecessary for a design to accommodate the same number of levels as the run size. However, there are few studies on the construction of space-filling designs with a large run size and a fixed number of levels. This paper will fill the gap between Latin hypercube designs and two-level fractional factorial designs and offer an algorithm for generating space-filling designs with flexible run sizes and numbers of levels.

The rest of this paper is organized as follows. Section 2 introduces the background and some notation, discussing several space-filling criteria, kernel functions and their connections. Section 3 provides general theoretical results for designs with Kronecker product structure. Section 4 proves that several commonly used criteria are kernel-based space-filling criteria. Section 5 discusses optimal designs with Kronecker product structure under the kernel-based space-filling criteria. Section 6 puts forward an algorithm to generate space-filling designs with flexible run sizes and numbers of levels. Section 7 concludes this paper. Some relevant results, all proofs, some additional comparisons and simulations, and a large table are provided in the supplementary material.

2. Space-filling Criteria and Kernel Function

In this section, we first introduce some definitions and notation. Then we discuss some commonly used space-filling criteria, the kernel function, and their connections.

Let $D(N, s^m) = (x_{ij})_{N\times m}$ denote a design with N rows, m columns and s levels, where x_{ij} belongs to $\mathcal{X} = \{-(s-1)/2, -(s-3)/2, \ldots, (s-1)/2\}$. A $D(N, s^m)$ is called a U-type design if each level appears equally often in each column. Furthermore, a $D(N, s^m)$ is called an orthogonal array of strength t, denoted by $OA(N, m, s, t)$, if every possible t-tuple occurs the same number of times in each of its $N \times t$ subarrays.

Let $H(n,2^q)=(h_{ij})_{n\times q}$ be a two-level design whose two levels are -1 and 1. In what follows, H is used to denote a matrix with entries only -1 and 1 unless otherwise stated. Let D be a $D(N,s^m)$ and H be an $H(n,2^q)$, then the Kronecker product of H and D is defined as

$$H\otimes D=\begin{pmatrix} h_{11}D & h_{12}D & \cdots & h_{1q}D \\ h_{21}D & h_{22}D & \cdots & h_{2q}D \\ \vdots & \vdots & & \vdots \\ h_{n1}D & h_{n2}D & \cdots & h_{nq}D \end{pmatrix}.$$

It is obvious that the elements of $H\otimes D$ are still in $\mathcal{X}$. For a $D(N,s^m)$, if its mirror image $-D$ is itself up to row permutations, we call it mirror-symmetric (Tang and Xu, 2014). If the correlation coefficient between any two distinct columns of a design is zero, the design is orthogonal.

2.1 Space-filling criteria

In this subsection, we review and introduce several commonly used criteria that can measure the space-filling property of a design. Different criteria evaluate the space-filling property of a design from different perspectives.

Maximin L_p-distance criterion. For a $D(N,s^m)$, let $d_p(\boldsymbol{x}_i,\boldsymbol{x}_j)=\sum_{k=1}^m|x_{ik}-x_{jk}|^p$ be the L_p-distance between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$, where $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are the ith and jth rows of D respectively. The maximin L_p-distance criterion is to maximize the minimal pairwise L_p-distance of D, denoted by $d_p(D)$. Zhou and Xu (2015) provided an upper bound of $d_p(D)$ for a U-type $D(N,s^m)$ as shown below.

Lemma 1 (Zhou and Xu, 2015)**.** *For any U-type $D(N,s^m)$, we have $d_2(D)\le\lfloor\bar{d}_2\rfloor$, where $\bar{d}_2=Nm(s^2-1)/(6N-6)$.*

Discrepancy. Discrepancies are proposed to measure the uniformity of a design through the difference between the empirical distribution function and the uniform distribution function, such as the centered L_2-discrepancy (CD), wrap-around L_2-discrepancy (WD), mixture discrepancy (MD), discrete discrepancy (DD) and Lee discrepancy (LD). For example, the squared CD of a $D(N, s^m)$ is defined as

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

Maximum projection criterion. Joseph, Gul and Ba (2015) proposed the maximum projection criterion for a $D(N, s^m)$, which is defined as

$$\psi(D) = \frac{2}{N(N-1)}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\prod_{k=1}^{m}\frac{1}{|x_{ik}-x_{jk}|^2}.$$

They referred to the design that minimizes $\psi(D)$ as a maximum projection design.

Generalized wordlength pattern. Xu and Wu (2001) defined $(A_1(D), \ldots, A_m(D))$ as the generalized wordlength pattern (GWLP) of a $D(N, s^m)$, where $A_k(D) = N^{-2}\sum_j \left(\sum_{i=1}^N x_{ij}^{(k)}\right)^2$ for $k = 1, \ldots, m$, and $G_k = \left(x_{ij}^{(k)}\right)$ is the matrix of orthonormal contrast coefficients for all its k-factor interactions under an ANOVA model. They also proposed the generalized minimum aberration (GMA) criterion, which minimizes $A_1(D), \ldots, A_m(D)$ sequentially, to rank different designs.

β-wordlength pattern. When considering a polynomial model for a $D(N, s^m)$, let α_k be the vector of all k-order interactions and $X_k = \left(x_{ij}^{(k)}\right)_{N\times n_k}$ be the matrix of orthonormal polynomial contrast coefficients for α_k, where n_k is the number of effects with order k. Cheng and Ye (2004) defined the β-wordlength pattern as $(\beta_1, \ldots, \beta_K)$, where $\beta_k(D) = N^{-2} \sum_{j=1}^{n_k} \left| \sum_{i=1}^{N} x_{ij}^{(k)} \right|^2$ for $k = 1, \ldots, K$, and $K = m(s-1)$. Similar to GMA, the minimum β-aberration criterion is to minimize $\beta_1(D), \ldots, \beta_K(D)$ sequentially.

Although GWLP and the β-wordlength pattern characterize a design from the perspective of factor aliasing, they can reflect the space-filling property of the design to a certain extent. For instance, Hickernell and Liu (2002) demonstrated that the GMA criterion can be defined and generalized by discrepancy. Ai and Zhang (2004) proved that the optimal designs under the GMA criterion possess favorable low-dimensional projection properties. Tang, Xu and Lin (2012) established that the CD and the β-wordlength pattern are exactly equivalent for a class of regular designs. Therefore, we incorporate the GMA and minimum β-aberration criteria into the scope of discussion in this paper.

Wordlength enumerator. For a $D(N, s^m)$, there is no explicit expression for the GMA and minimum β-aberration criteria. To address this issue, Tang and Xu (2021) defined $E_\alpha(D, z) = \sum_{k=0}^{m} A_k(D) z^k$ and $E_\beta(D, z) = \sum_{k=0}^{m(s-1)} \beta_k(D) z^k$. When $z \to 0$, minimizing $E_\alpha(D, z)$ and minimizing $E_\beta(D, z)$ are equivalent to the GMA and minimum β-aberration criteria, respectively. Furthermore, by proposing the wordlength enumerator $E(D) = N^{-2} \sum_{i=1}^{N} \sum_{j=1}^{N} \prod_{k=1}^{m} \sum_{l=0}^{s-1} p_l(x_{ik}) p_l(x_{jk}) z_l$, where $\{p_0(x)$, $p_1(x)$, …, $p_{s-1}(x)\}$ is an orthogonal polynomial basis and $z_l \geq 0$, they unified $E_\alpha(D, z)$ and $E_\beta(D, z)$. In the following, we only consider the wordlength enumerator and no longer discuss the GMA and minimum β-aberration criteria separately.

2.2 Kernel function

In this subsection, we introduce the definition of kernel function, and then discuss its connection with a class of space-filling criteria.

Definition 1. A function $f : \mathcal{X} \times \mathcal{X} \to R$ is called a kernel function on $\mathcal{X}$ if and only if it satisfies that: (a) f is symmetric in the variables, i.e., $f(x, y) = f(y, x)$ holds for any $x, y \in \mathcal{X}$; and (b) for any positive integer $n \leq s$ and $w_i \in R$, distinct $x_i \in \mathcal{X}$ for $i = 1, \ldots, n$, $\sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j f(x_i, x_j) \geq 0$.

Assume that a space-filling criterion for a $D(N, s^m)$ has the following form

$$\phi(D) = \sum_{i=1}^{N} \sum_{j=1}^{N} w_i w_j \prod_{k=1}^{m} f_k(x_{ik}, x_{jk}),$$

where w_i can be regarded as the weight of the ith point in the design D and $f_k(x, y)$ can be regarded as the criterion used to evaluate the space-filling property of the kth factor. For example, we can assign larger weights to the points in the central region than those in the boundary region if we need to pay more attention to the central region. We are free to choose the kernel function for the kth factor. For example, we can use a kernel function corresponding to the maximum projection criterion for quantitative factors, and a kernel function corresponding to the wordlength enumerator for qualitative factors.

As a reasonable space-filling criterion, symmetrically reflecting all design points about the origin should keep the value of $\phi(D)$ unchanged. Therefore, $f_k(x, y)$ should be symmetric about the origin, i.e., $f_k(x,y) = f_k(-x,-y)$ holds for any $x, y \in \mathcal{X}$ and $k = 1, \ldots, m$. When we have no prior information, it is natural to take $w_i = 1/N$ for $i = 1, 2, \ldots, N$ and $f_1 = f_2 = \cdots = f_k = f$, i.e.,

$$\phi(D) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} F(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \prod_{k=1}^{m} f(x_{ik}, x_{jk}), \tag{2.1}$$

where $F(\boldsymbol{x}_i, \boldsymbol{x}_j) = \prod_{k=1}^{m} f(x_{ik}, x_{jk})$. Actually, many space-filling criteria can be written in the form of (2.1). For example, if $f(x,y) = 1 + |x|/(2s) + |y|/(2s) - |x-y|/(2s)$, then $f(x,y)$ is the reproducing kernel corresponding to CD. In this case, $\phi(D)$ is the double summation term of CD^2. If $f(x,y) = 1/|x-y|^2$, then $f(x,y)$ is also a kernel function and $\phi(D)$ corresponds to the maximum projection criterion. In most cases, the goal is to minimize the value of $\phi(D)$.

Zhou and Xu (2014) proposed a general space-filling criterion with the same form as (2.1), and calculated the average of the criterion values over all level permutations of a design. In this paper, we derive the expression for designs with Kronecker product structures under this criterion. Due to the differences in computational objectives, there exist significant differences in our constraints on $f(x,y)$ compared with those imposed by Zhou and Xu (2014), i.e., we require $f(x,y)$ to be a kernel function symmetric about the origin, while Zhou and Xu (2014) required $f(x,y)$ to satisfy $f(x,y) \geq 0$ and $f(x,x) + f(y,y) > f(x,y) + f(y,x)$ for any $x \neq y$. Furthermore, Zhou and Xu (2014) only considered the L_2-discrepancies and the extended maximin distance criterion, whereas we will additionally consider the maximum projection criterion and the wordlength enumerator.

Hereafter, $\phi(D)$ is assumed to have the form of (2.1). A criterion is called a kernel-based space-filling criterion if it can be written in the form of $\phi(D)$ in (2.1) with a kernel function $f(x,y)$ on $\mathcal{X}$. Note that, for the maximum projection criterion, there may exist cases where the denominator is 0, which does not affect our results. The specific details will be discussed in Section 4. Unfortunately, it seems that a few commonly used criteria cannot be written in the form of (2.1), such as the distance variance and mean squared correlation criteria. We will discuss them in the supplementary material.

3. General Theoretical Results

In this section, we provide theoretical results for designs with Kronecker product structure. Kronecker product is powerful for constructing designs with good space-filling property. Example 1 demonstrates an optimal design with a Kronecker product structure under the maximin L_2-distance criterion.

Example 1. Let

$$D = \begin{pmatrix} 0.5 & 1.5 & 0.5 & 1.5 & -0.5 & -1.5 & -0.5 & -1.5 \\ 1.5 & -0.5 & 1.5 & -0.5 & -1.5 & 0.5 & -1.5 & 0.5 \\ 0.5 & 1.5 & -0.5 & -1.5 & 0.5 & 1.5 & -0.5 & -1.5 \\ 1.5 & -0.5 & -1.5 & 0.5 & 1.5 & -0.5 & -1.5 & 0.5 \end{pmatrix}^T$$

be a $D(8,4^4)$ with $d_2(D)=10$. It is constructed using the method presented in Section 5.2 by taking the Kronecker product of two designs

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix}^T \text{ and } \begin{pmatrix} 0.5 & 1.5 \\ 1.5 & -0.5 \end{pmatrix}.$$

Furthermore, it can be proved to be optimal under the maximin L_2-distance criterion (See Table 2).

Example 1 shows that the design with Kronecker product structure may perform well under the maximin L_2-distance criterion. Therefore, we believe that some designs with Kronecker product structure exhibit good space-filling properties. In this paper, we consider the designs with a more general form defined as

$$D_0 = H \otimes D, \tag{3.1}$$

where D is a $D(N, s^m)$ and H is an $H(n, 2^q)$ with $n \geq 2$. The construction method in (3.1) has been studied in several existing works. For example, Bingham, Sitter and Tang (2009) investigated the orthogonality of designs obtained from (3.1); Lin et al. (2010) proposed a method for constructing orthogonal Latin hypercube designs based on this formulation. Theorem 1 provides an expression of $\phi(D_0)$ in terms of GWLP.

Theorem 1. *For a ϕ with the form of (2.1), where $f(x,y)$ is symmetric both in the variables and about the origin, then we have $\phi(D_0) = \sum_{g=0}^{q} C(D,g,q)A_g(H)$, where $(A_0(H), A_1(H), \ldots, A_q(H))$ is the GWLP of H and*

$$C(D,g,q) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{F(\boldsymbol{x}_i,\boldsymbol{x}_j)+F(\boldsymbol{x}_i,-\boldsymbol{x}_j)}{2}\right)^{q-g}\left(\frac{F(\boldsymbol{x}_i,\boldsymbol{x}_j)-F(\boldsymbol{x}_i,-\boldsymbol{x}_j)}{2}\right)^{g}. \tag{3.2}$$

It is worth noting that, besides the symmetry about the origin, we only require that $f(x,y)$ is symmetric in the variables in the theorem, not necessary to be a kernel function on $\mathcal{X}$. According to Theorem 1, the value of $\phi(D_0)$ is determined by $C(D,g,q)$ and $A_g(H)$ which are related to D and H respectively. The following example illustrates how to calculate $\phi(D_0)$ using Theorem 1.

Example 2. Let $D(8,4^4)$ be the D in Example 1 and $H(4,2^3) = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}^T$.

It is easy to verify that $(A_0(H), A_1(H), A_2(H), A_3(H)) = (1, 0, 0, 1)$. If we choose $f(x, y) = 1 + |x|/8 + |y|/8 - |x - y|/8$, we can get $(C(D, 0, 3), C(D, 1, 3), C(D, 2, 3), C(D, 3, 3)) = (3.1595, 0, 0.2057, 0)$. Thus, we have $\phi(H \otimes D) = C(D, 0, 3) = 3.1595$, which is consistent with the results obtained by calculating $\phi(H \otimes D)$ directly.

In order to minimize $\phi(D_0)$, the selection of H depends on the signs and relative sizes of $C(D, g, q)$'s. For example, if $C(D, g, q)$ is positive and decreases as g increases, we prefer an H which minimizes $A_1(H), A_2(H), \ldots, A_q(H)$ sequentially. Therefore, we will focus more on the properties of $C(D, g, q)$. According to Theorem 1, the following corollary can be immediately obtained.

Corollary 1. *If D is mirror-symmetric, then $C(D, g, q) = 0$ holds for any odd g, where $C(D, g, q)$ is defined by* (3.2).

Remark 1. As shown in Example 2, it may not be true that $C(D, g_1, q) \geq C(D, g_2, q)$ for any $g_1 < g_2$. For example, according to Corollary 1, $C(D, g, q) = 0$ for any odd g and $C(D, g, q) > 0$ for any even g when D is mirror-symmetric.

$A_g(H)$ characterizes the degree of factor aliasing for design H. Thus, a design with a smaller value of $A_g(H)$ is more preferable. Based on this, for a reasonable space-filling criterion, a natural requirement is that all $C(D, g, q)$ be nonnegative. For example, if $C(D, 1, 1)$ is negative for some D and $f(x, y)$, and H has only one column, then $\phi(D_0) = C(D, 0, 1) + A_1(H)C(D, 1, 1)$ according to Theorem 1. Therefore, $A_1(H)$ should be as large as possible. As is well known, $A_1(H)$ is maximized when the entries of H are either all 1 or all -1, which implies that the design obtained by repeating the points in D or $-D$ performs better than that with other choices of H. This violates the fundamental requirement of the space-filling criterion, since the space-filling property requires that design points explore the entire experimental space as much as possible and avoid duplicate points as far as possible.

Remark 2. To ensure the nonnegativity of $C(D, g, q)$, it is not sufficient for $f(x, y)$ to only satisfy the conditions in Theorem 1. For example, for $f(x, y) = |x - y|$ which satisfies the conditions in Theorem 1, we have $C(D, 1, 1) < 0$ if D has only one row with all elements nonzero.

The following theorem states that if $f(x, y)$ is further a kernel function, then all the coefficients $C(D, g, q)$ of $A_g(H)$ defined by (3.2) in Theorem 1 are nonnegative for any $D(N, s^m)$, q and $g = 0, 1, \ldots, q$.

Theorem 2. *If ϕ is a kernel-based space-filling criterion with $f(x, y)$ being symmetric about the origin, then $C(D, g, q) \geq 0$ for any $D(N, s^m)$, q and $g = 0, 1, \ldots, q$, where $C(D, g, q)$ is defined by* (3.2).

In the next section, we will investigate whether the criteria mentioned in Section 2 are kernel-based space-filling criteria and provide the corresponding theoretical justifications.

4. Kernel-based Space-filling Criterion

In this section, our main goal is to prove that several commonly used space-filling criteria are kernel-based space-filling criteria.

4.1 Results under L_2-type discrepancies

In this subsection, we explore the property of $C(D,g,q)$ defined by (3.2) when $f(x,y)$ corresponds to the double summation term of an L_2-type discrepancy. For a $D(N,s^m)$ and a kernel function $f(x,y)$ on $[-s/2,s/2]$, let $F(\boldsymbol{x},\boldsymbol{y}) = \prod_{k=1}^m f(x_k,y_k)$ with $\boldsymbol{x}=(x_1,\ldots,x_m)^T$ and $\boldsymbol{y}=(y_1,\ldots,y_m)^T$. The L_2-type discrepancy of D is defined as

$$\begin{aligned}\mathrm{Disc}^2(D,F) = &\int_{\mathcal{W}\times\mathcal{W}} F(\boldsymbol{x},\boldsymbol{y})dF_{\mathrm{u}}(\boldsymbol{x})dF_{\mathrm{u}}(\boldsymbol{y}) - \frac{2}{N}\sum_{i=1}^N \int_{\mathcal{W}} F(\boldsymbol{x}_i,\boldsymbol{y})\,dF_{\mathrm{u}}(\boldsymbol{y}) \\ &+ \frac{1}{N^2}\sum_{i=1}^N\sum_{j=1}^N F(\boldsymbol{x}_i,\boldsymbol{x}_j),\end{aligned}$$

where $\mathcal{W}=[-s/2,s/2]^m$ and $F_{\mathrm{u}}(\cdot)$ is the uniform distribution on $\mathcal{W}$. Here are some commonly used examples of kernel functions for L_2-type discrepancies. (a) For CD, the kernel function is $f(x,y)=1+|x|/(2s)+|y|/(2s)-|x-y|/(2s)$; (b) For WD, the kernel function is $f(x,y)=3/2-|x-y|/s+|x-y|^2/s^2$; (c) For MD, the kernel function is $f(x,y)=15/8-|x|/(4s)-|y|/(4s)-3|x-y|/(4s)+|x-y|^2/(2s^2)$; (d) For DD, the kernel function is $f(x,y)=a$ if $x=y$, or b if $x\neq y$, where a and b satisfy that $-a/(s-1)<b<a$; (e) For LD, the kernel function is $f(x,y)=1-\min\{1-|x-y|,|x-y|\}$.

When we choose any of the kernel functions above, $\phi(D)$ is equal to the third term in $\mathrm{Disc}^2(D,F)$. It can be verified that all kernel functions mentioned above are symmetric about the origin, and therefore the corresponding $C(D,g,q)$'s are all nonnegative. The first term of $\mathrm{Disc}^2(D,F)$ is a constant that only depends on the number of columns in D. For design $H\otimes D$ with D being a fixed $D(N,s^m)$, the values of the second term in $\mathrm{Disc}^2(H\otimes D,F)$ only depends on the column size of H. Therefore, we can obtain the following corollary.

Corollary 2. *Let* $D_1 = (D^T, -D^T)^T$*, then we have* $\mathrm{Disc}^2(D_1, F) \leq \mathrm{Disc}^2(D, F)$ *if* f *represents CD, WD, MD, DD or LD, where* $F(\boldsymbol{x}, \boldsymbol{y}) = \prod_{k=1}^{m} f(x_k, y_k)$.

Corollary 2 is an interesting and intuitive result from Theorem 2. In other words, if the mirror image of a design D is juxtaposed with itself, then its CD, WD, MD, DD and LD will definitely not increase.

4.2 Results under the wordlength enumerator

As mentioned earlier, the wordlength enumerator can reflect the space-filling property of a design to a certain extent. In this subsection, we discuss the relevant results when $f(x, y)$ corresponds to the wordlength enumerator.

For $x, y \in \mathcal{X}$, let $f(x, y) = \sum_{l=0}^{s-1} p_l(x) p_l(y) z_l$, where $\{p_0(x), p_1(x), \ldots, p_{s-1}(x)\}$ is an orthogonal polynomial basis and $z_l \geq 0$. For this function, the corresponding $\phi(D)$ is exactly the wordlength enumerator of D. According to Theorems 1 and 2 in Tang and Xu (2021), we have the following lemma.

Lemma 2. *For a* $D(N, s^m)$*, we have* (a) $\phi(D) = \sum_{k=0}^{m} A_k(D) z^k$ *if* $z_l = z$*; and* (b) $\phi(D) = \sum_{k=0}^{m(s-1)} \beta_k(D) z^k$ *if* $z_l = z^l$.

According to the properties of orthogonal polynomial basis, $p_l(-x) = p_l(x)$ for an even l and $p_l(-x) = -p_l(x)$ for an odd l. It is straightforward to verify that $f(x, y)$ is symmetric about the origin. In addition, it is a kernel function on $\mathcal{X}$ by noting that

$$\begin{aligned}\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j f(x_i, x_j) &= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \sum_{l=0}^{s-1} p_l(x_i) p_l(x_j) z_l = \sum_{l=0}^{s-1} z_l \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j p_l(x_i) p_l(x_j) \\ &= \sum_{l=0}^{s-1} z_l \left(\sum_{i=1}^{n} c_i p_l(x_i) \right)^2 \geq 0.\end{aligned}$$

Therefore, the following corollary is evident.

Corollary 3. *Let* $f(x,y)=\sum_{l=0}^{s-1}p_l(x)p_l(y)z_l$, *where* $\{p_0(x),p_1(x),\ldots,p_{s-1}(x)\}$ *is an orthogonal polynomial basis and* $z_l\geq 0$, *we have* $C(D,g,q)\geq 0$ *for any* D, q *and* $g=0,1,\ldots,q$, *where* $C(D,g,q)$ *is defined by* (3.2).

For the D_0 defined in (3.1), we can calculate $A_k(D_0)$ for $k=1,2,\ldots,mq$ and $\beta_k(D_0)$ for $k=1,2,\ldots,mq(s-1)$ according to Theorem 1. In particular, the following corollary provides the explicit expressions of $A_1(D_0)$ and $\beta_1(D_0)$.

Corollary 4. *For* $D_0=H\otimes D$ *defined in* (3.1) *with* $D=(x_{ik})_{N\times m}$, *we have*

$$\begin{aligned}
A_1(D_0) &= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{m}\left\{\sum_{\substack{1\leq l\leq s-1,\\ l\text{ is odd}}}p_l(x_{ik})p_l(x_{jk})+qA_1(H)\sum_{\substack{1\leq l\leq s-1,\\ l\text{ is even}}}p_l(x_{ik})p_l(x_{jk})\right\},\ \textit{and}\\
\beta_1(D_0) &= \beta_1(D)A_1(H).
\end{aligned}$$

Corollary 4 is derived from Theorem 1, and it enables us to evaluate the one-dimensional projection property of the resulting design. In addition, if D is a two-level design and the obtained D_0 is taken as H in (3.1) again, this corollary allows us to directly calculate $A_1(H)$.

4.3 Results under adjusted maximum projection criterion

In this subsection, we discuss the theoretical results when $f(x,y)$ corresponds to the maximum projection criterion, i.e., $f(x,y)=1/|x-y|^2$. In this case, we have $\phi(D)=N^{-2}\sum_{i=1}^{N}\sum_{j=1}^{N}\prod_{k=1}^{m}1/|x_{ik}-x_{jk}|^2$. To avoid the denominator being zero and maintain consistency of ϕ with (2.1), we make some adjustments to $f(x,y)$ by taking

$f(x, y) = 1/(\gamma + |x - y|)^2$ for $\gamma > 0$ as Joseph, Gul and Ba (2019) suggested. Moreover, Joseph (2016) indicated that the squares in $f(x, y)$ can be replaced by $l \geq 1$, that is,

$$f(x, y) = 1/(\gamma + |x - y|)^l \tag{4.1}$$

for $\gamma > 0$. Hence, the adjusted maximum projection criterion is defined as $\phi(D) = N^{-2} \sum_{i=1}^{N} \sum_{j=1}^{N} \prod_{k=1}^{m} 1/(\gamma + |x_{ik} - x_{jk}|)^l$ for a small $\gamma > 0$. When $\gamma \to 0$, $\phi(D)$ is equivalent to the maximum projection criterion.

It is obvious that the $f(x, y)$ in (4.1) is symmetric both in the variables and about the origin. Generally, for ease of computation, it is common to choose $l = 1$ or $l = 2$. The following theorem shows that the adjusted maximum projection criterion is a kernel-based space-filling criterion when $l = 1$ or $l = 2$. Thus, the corresponding $C(D, g, q)$'s are all nonnegative.

Theorem 3. *Let $f(x, y) = 1/(\gamma + |x - y|)^l$ for $\gamma \geq 0$ with $l = 1$ or $l = 2$, then $f(x, y)$ is a kernel function on $\mathcal{X}$.*

4.4 Results under extended maximin distance criterion

Zhou and Xu (2014) proposed an extended form of the maximin L_p-distance criterion as $\chi(D) = N^{-2} \sum_{i=1}^{N} \sum_{j=1}^{N} \rho^{d_p(\boldsymbol{x}_i, \boldsymbol{x}_j)}$ for $0 < \rho < 1$. When $\rho \to 0$, minimizing $\chi(D)$ implies maximizing the $d_p(D)$ of a $D(N, s^m)$. It is called an extended maximin L_p-distance criterion because it further minimizes the number of point pairs that achieve the minimal pairwise L_p-distance.

In this subsection, we choose $f(x, y) = \rho^{d_p(x,y)}$, where $d_p(x, y) = |x - y|^p$ and

$0 < \rho < 1$, then $\phi(D)$ in (2.1) can be expressed as $\phi(D) = N^{-2}\sum_{i=1}^{N}\sum_{j=1}^{N}\rho^{d_p(\boldsymbol{x}_i,\boldsymbol{x}_j)}$. Let $B_j(D) = N^{-1}\text{card}\{(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{x},\boldsymbol{y} \in D \text{ and } d_p(\boldsymbol{x},\boldsymbol{y}) = j\}$ for $j = 0, 1, \ldots, M$, where card$\{\cdot\}$ denotes the cardinality of a set and $M = m(s-1)^p$. Zhou and Xu (2014) proposed to minimizing $B_0(D), B_1(D), \ldots, B_M(D)$ sequentially. When the design has no repeated points, it is obvious that $B_0(D) = 1$ and the minimum distance of the design D is $\min\{k \in Z^+ : B_k(D) > 0\}$.

In fact, we have $\phi(D) = (1/N)\sum_{k=1}^{M}\rho^k B_k(D)$ and minimizing $\phi(D)$ is equivalent to sequentially minimizing $B_0(D), B_1(D), \ldots, B_M(D)$ when $\rho \to 0$. The following theorem shows that the extended maximin distance criterion is a kernel-based space-filling criterion under some conditions. Thus, all corresponding $C(D, g, q)$'s are nonnegative.

Theorem 4. *Suppose that $d_p(x, y) = |x - y|^p$ and $f(x, y) = \rho^{d_p(x,y)}$, then $f(x, y)$ is a kernel function on $\mathcal{X}$ for $0 < \rho \leq 1/3$ and $p \geq 1$. Furthermore, if $p = 1$ or $p = 2$, $f(x, y)$ is a kernel function on $\mathcal{X}$ for $0 < \rho < 1$.*

It should be noted that the first part of Theorem 4 is derived from the monotonicity of $|x - y|^p$, while the second part is obtained from the specific forms when $p = 1$ and $p = 2$. This difference in derivation leads to distinct ranges of ρ in the respective results. Given that $p = 1$ and $p = 2$ are the most practically relevant cases, the second part of the theorem retains significant practical and theoretical value.

Combining all the results obtained in this section, we have proved that $C(D, g, q)$ is nonnegative under the space-filling criteria above. Although $C(D, g, q)$ may not decrease as g increases, D_0 tends to have good performance under these criteria when H minimizes $A_1(H), \ldots, A_q(H)$ sequentially.

5. Optimal Designs with Kronecker Product Structures

For a given criterion, it is desirable to obtain designs that perform well under it. In this section, we provide optimal designs with Kronecker product structures under a class of space-filling criteria. Specifically, we examine the corresponding optimality results under the maximin L_2-distance criterion, which is one of the most widely used space-filling criteria.

5.1 Optimal designs under kernel-based space-filling criterion

According to Theorem 1, we have $\phi(D_0) = \sum_{g=0}^{q} C(D,g,q)A_g(H)$ under some conditions. However, it is a highly challenging task to find a D that minimizes $\phi(D_0)$ when the values of $A_g(H)$ are unknown for $g = 1, 2, \ldots, q$. Therefore, we consider a specific case of H, namely a two-level full factorial design. Let H_q be a two-level full factorial design with q factors, for example, $H_1 = (1, -1)^T$ and $H_2 = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix}^T$. For $D_0 = H_q \otimes D$ with D being a $D(N, s^m)$, we have

$$\phi(D_0) = C(D,0,q) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{F(\boldsymbol{x}_i, \boldsymbol{x}_j) + F(\boldsymbol{x}_i, -\boldsymbol{x}_j)}{2}\right)^q.$$

Let $P_1 = \prod_{i \neq j,\, i,j \in \mathcal{X}} f(i,j), P_2 = \prod_{i \neq j,\, i,j \in \mathcal{X}} f(i,-j), Q_1 = \prod_{i \in \mathcal{X}} f(i,i)$, and $Q_2 = \prod_{i \in \mathcal{X}} f(i,-i)$. Theorem 5 gives a lower bound of $\phi(D_0)$ with $D_0 = H_q \otimes D$.

Theorem 5. *Let D be a U-type $D(N, s^m)$, H_q be a two-level full factorial design, and $D_0 = H_q \otimes D$, then we have $\phi(D_0) \geq LW_1$ for a ϕ with the form of (2.1), where*

$$LW_1 = \frac{1}{N}\left(\frac{Q_1^{\frac{m}{s}} + Q_2^{\frac{m}{s}}}{2}\right)^q + \frac{N-1}{N}\left(\frac{P_1^{\frac{Nm}{s^2(N-1)}} Q_1^{\frac{(N-s)m}{s^2(N-1)}} + P_2^{\frac{Nm}{s^2(N-1)}} Q_2^{\frac{(N-s)m}{s^2(N-1)}}}{2}\right)^q.$$

The equality holds if $F(\boldsymbol{x}_i, \boldsymbol{x}_j)$ keeps the same for any $i \neq j$, $i, j = 1, \ldots, N$, so do $F(\boldsymbol{x}_i, -\boldsymbol{x}_j)$ for $i \neq j$, $i, j = 1, \ldots, N$, $F(\boldsymbol{x}_i, \boldsymbol{x}_i)$ for $i = 1, \ldots, N$, and $F(\boldsymbol{x}_i, -\boldsymbol{x}_i)$ for $i = 1, \ldots, N$, where $\boldsymbol{x}_i$ is the ith row of D.

Fortunately, component orthogonal array (COA) is closely related to the equality conditions stated in Theorem 5. A $D(N_1, s^{m_1})$ is called a COA if each row is a permutation of all levels and, for any two columns, each level combination (i, j) with $i \neq j$ and $i, j \in \mathcal{X}$ appears equally often. For the construction methods of COA, one can refer to Yang, Sun and Xu (2021). It can be easily verified that if D^T is a COA, then D satisfies the equality conditions stated in Theorem 5. The following example provides a COA and explains its optimality.

Example 3. Let $f(x, y) = 0.7^{|x-y|}$ and

$$D = \begin{pmatrix} -1.5 & -1.5 & -1.5 & -0.5 & -0.5 & -0.5 & 0.5 & 0.5 & 0.5 & 1.5 & 1.5 & 1.5 \\ -0.5 & 0.5 & 1.5 & -1.5 & 1.5 & 0.5 & 1.5 & -1.5 & -0.5 & 0.5 & -0.5 & -1.5 \\ 0.5 & 1.5 & -0.5 & 1.5 & 0.5 & -1.5 & -1.5 & -0.5 & 1.5 & -0.5 & -1.5 & 0.5 \\ 1.5 & -0.5 & 0.5 & 0.5 & -1.5 & 1.5 & -0.5 & 1.5 & -1.5 & -1.5 & 0.5 & -0.5 \end{pmatrix}.$$

Then D^T is a COA with 12 rows and 4 columns. If $q = 2$, $D_0 = H_2 \otimes D$ is a U-type $D(16, 4^{24})$ with $\phi(D_0) = LW_1 = 0.06256$. If $q = 3$, $D_0 = H_3 \otimes D$ is a U-type $D(32, 4^{36})$ with $\phi(D_0) = LW_1 = 0.03127$. If $q = 4$, $D_0 = H_4 \otimes D$ is a U-type $D(64, 4^{48})$ with $\phi(D_0) = LW_1 = 0.01564$.

Although we have proven that D_0 achieves the lower bound LW_1 when D is the transpose of a COA, COA is restricted by its inherent properties, resulting in certain limitations on the numbers of rows and columns of D_0. For example, for a COA with N_1 rows and m_1 columns, N_1 must be an integer multiple of $m_1(m_1 - 1)$. Besides the transpose of COA, we discuss two additional classes of designs that also satisfy the equality condition in Theorem 5.

The first class is the U-type full design, which can be constructed using the following method. For fixed N and s, we obtain a design D by generating all possible combinations of the set $\{0, 1, \ldots, s-1\}$ with each element repeating $\alpha = N/s$ times in each column. Then D is a U-type $D(N, s^m)$ with $m = N!/(\alpha!)^s$. The other class consists of the transposes of Type II orthogonal arrays with strength 2 (OAII). Rao (1961) defined OAII by simply replacing the term "level combination (i, j)" in the COA definition with "unordered pairs (i, j)", and provided the corresponding construction method. For example,

$$D = \begin{pmatrix} -2 & -2 & -1 & -1 & 0 & 0 & 1 & 1 & 2 & 2 \\ 2 & 1 & -2 & 2 & -1 & -2 & 0 & -1 & 1 & 0 \\ 1 & -1 & 2 & 0 & -2 & 1 & -1 & 2 & 0 & -2 \\ 0 & 2 & 1 & -2 & 2 & -1 & -2 & 0 & -1 & 1 \\ -1 & 0 & 0 & 1 & 1 & 2 & 2 & -2 & -2 & -1 \end{pmatrix}$$

is the transpose of an OAII. It is straightforward to verify that the above two classes of designs both satisfy the equality condition in Theorem 5.

Table 1 presents the numbers of rows (N_1), columns (m_1) and levels (s_1) of the COAs, OAIIs and U-type full designs (Full) that can be used, as well as the numbers of rows (N_0), columns (m_0) and levels (s_1) of the resulting designs with Kronecker product structures achieving LW_1. All numbers m are prime powers, except that OAIIs require m to be an odd prime power, with α, λ and n being positive integers.

Table 1: Designs achieving the lower bound LW_1.

N_1	m_1	s_1	N_0	m_0	Type
$\lambda m(m-1)^{\dagger}$	m	m	$m2^q$	$\lambda qm(m-1)$	COA
$\lambda(m+n)!/(m-2)!^{\ddagger}$	$m+n$	$m+n$	$(m+n)2^q$	$\lambda q(m+n)!/(m-2)!$	COA
$60^{\S}$	6	6	6×2^q	$60q$	COA
$90^{\S}$	6	6	9×2^q	$90q$	COA
$\lambda m(m-1)/2^{\sharp}$	m	m	$m2^q$	$\lambda qm(m-1)/2$	OAII
αs	$(\alpha s)!/(\alpha!)^s$	s	$(\alpha s)!/(\alpha!)^s 2^q$	$q\alpha s$	Full

†: designs from Yang, Sun and Xu (2021); ‡: designs from Huang (2021);
§: designs from Zhao, Li and Zhao (2021); ♯: designs from Rao (1961).

Even if D_0 reaches the lower bound LW_1, it does not necessarily guarantee the optimality among all U-type designs with the same size of D_0. For ease of comparison, we set the number of rows of D as $N2^q$ and the number of columns as mq. Theorem 6 provides a lower bound for $\phi(D)$ when D is an arbitrary U-type $D(N2^q, s^{mq})$.

Theorem 6. *Let $n = 2^q$ and D be a U-type $D(Nn, s^{mq})$, then we have $\phi(D) \geq LW_2$ for a ϕ with the form of* (2.1), *where*

$$LW_2 = \frac{1}{N}\left(\frac{Q_1^{\frac{m}{s}}}{2}\right)^q + \frac{Nn-1}{Nn} P_1^{\frac{Nnmq}{s^2(Nn-1)}} Q_1^{\frac{(Nn-s)mq}{s^2(Nn-1)}}.$$

It is obvious that $LW_2/LW_1 \leq 1$. Due to $P_1Q_1 = P_2Q_2$, we have $LW_2/LW_1 \to 1$ when $N \to \infty$ and $n \to \infty$. Therefore, if $\phi(D_0)$ reaches the lower bound LW_1, then it will be close to LW_2. Therefore, such a D_0 is a good space-filling design. The following example illustrates that D_0 exhibits high efficiency among all U-type designs with the same size.

Example 4 (Example 3 continued)**.** Let $f(x, y) = 0.7^{|x-y|}$ and D be the design in

Example 3. If $q = 2$, D_0 is a U-type $D(16, 4^{24})$ with $\phi(D_0) = LW_1 = 0.06256$ and $LW_2/LW_1 = 99.91\%$. If $q = 3$, D_0 is a U-type $D(32, 4^{36})$ with $\phi(D_0) = LW_1 = 0.03127$ and $LW_2/LW_1 = 99.94\%$. If $q = 4$, D_0 is a U-type $D(64, 4^{48})$ with $\phi(D_0) = LW_1 = 0.01564$ and $LW_2/LW_1 = 99.92\%$. Thus, we have enough reasons to believe that these designs perform well among all U-type designs with the same size.

It should be noted that when H is a two-level full factorial design H_q, the designs obtained from (3.1) are only available for certain combinations of run size and number of columns. Specifically, the run size must be a multiple of 2^q, and the number of columns must be a multiple of q.

5.2 Optimal designs under maximin L_2-distance criterion

In this subsection, we focus on the construction of optimal designs with Kronecker product structure under the maximin L_2-distance criterion. For convenience of expression, let $\delta(\boldsymbol{h}_i, \boldsymbol{h}_j) = \text{card}\{h_{ik} \neq h_{jk}, k = 1, 2, \ldots, q\}$ be the Hamming distance between two rows $\boldsymbol{h}_i$ and $\boldsymbol{h}_j$ in H and $\delta(H) = \min_{i \neq j}\{\delta(\boldsymbol{h}_i, \boldsymbol{h}_j)\}$. Let $d_o(D) = \min_{i}\{d_2(\boldsymbol{x}_i, 0)\}$, where $\boldsymbol{x}_i$ is the ith row of D and $d_2(\boldsymbol{x}_i, 0)$ is the L_2-distance between $\boldsymbol{x}_i$ and the origin. Let $\langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle = \sum_{k=1}^{m} x_{ik}x_{jk}$ be the inner product of $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. Theorem 7 provides an achievable upper bound of minimal pairwise L_2-distance for D_0.

Theorem 7. *For D_0 defined in (3.1), if D_0 is a U-type design, we have*

$$d_2(D_0) \leq \frac{mq(s^2 - 1)}{6}. \tag{5.1}$$

According to Lemma 1, the upper bound of minimal pairwise L_2-distance of any U-type $D(Nn, s^{mq})$ is $\lfloor \bar{d}_2 \rfloor = \lfloor Nnmq(s^2-1)/(6Nn-6) \rfloor$. Define $d_{eff}(D_0) = d_2(D_0)/\lfloor \bar{d}_2 \rfloor$ as the distance efficiency of design D_0. If $d_2(D_0)$ reaches the upper bound on the right-hand side of Inequality (5.1), then $d_{eff}(D_0) \to 1$ when $n \to \infty$ or $N \to \infty$. In the following, we will provide construction methods for H and D, such that the resulting D_0 can achieve the upper bound in Theorem 7.

For a U-type design D_0, the proof of Theorem 7 in the supplementary material implies that $d_2(D_0)$ achieves the upper bound on the right-hand side of (5.1) if H and D satisfy the following conditions: (i) $d_o(D) = m(s^2-1)/12$; (ii) $\langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle = 0$ for any two distinct rows $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ of D; (iii) $(D^T, -D^T)^T$ is a U-type design; (iv) H is a U-type design; (v) $\delta(H) \geq q/2$. Conditions (i), (ii) and (iii) are for D and Conditions (iv) and (v) are for H. Next we will illustrate how to construct D and H that satisfy the above conditions respectively. For two square matrices $A = (a_{ij})_{m\times m}$ and $B = (b_{ij})_{m\times m}$, define the Hadamard product of A and B as $A \circ B = (a_{ij}b_{ij})_{m\times m}$. The following construction method generates designs which satisfy Conditions (i), (ii) and (iii).

Construction 1.

Step 1. *Let* $H^{(1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ *and* $H^{(k)} = \begin{pmatrix} H^{(k-1)} & \tilde{H}^{(k-1)} \\ H^{(k-1)} & -\tilde{H}^{(k-1)} \end{pmatrix}$ *for* $k = 2, 3, \ldots,$

where $\tilde{H}^{(k-1)} = H^{(k-1)} \begin{pmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \iddots & \vdots & \vdots \\ 1 & \cdots & 0 & 0 \end{pmatrix}$.

Step 2. *Let* $A^{(1)} = \begin{pmatrix} 0.5 & 1.5 \\ 1.5 & 0.5 \end{pmatrix}$ *and* $A^{(k)} = \begin{pmatrix} A^{(k-1)} & A^{(k-1)} + 2^{k-1} \\ A^{(k-1)} + 2^{k-1} & A^{(k-1)} \end{pmatrix}$.

Step 3. *Let* $G^{(k)} = H^{(k)} \circ A^{(k)}$ *for* $k = 1, 2, \ldots$.

Proposition 1. *The $G^{(k)}$ obtained by Construction 1 satisfies Conditions* (i), (ii) *and* (iii).

In fact, the $G^{(k)}$ obtained by Construction 1 has the following properties: (a) $G^{(k)}$ is a $D(2^k, (2^{k+1})^{2^k})$; (b) any row or column is a signed permutation of $1/2, 3/2, \ldots, (2^{k+1}-1)/2$; (c) $(G^{(k)})^T G^{(k)}$ is proportional to I_{2^k}. For example, when $k = 3$, we have

$$G^{(3)} = \begin{pmatrix} 0.5 & 1.5 & 2.5 & 3.5 & 4.5 & 5.5 & 6.5 & 7.5 \\ 1.5 & -0.5 & -3.5 & 2.5 & 5.5 & -4.5 & -7.5 & 6.5 \\ 2.5 & 3.5 & -0.5 & -1.5 & -6.5 & -7.5 & 4.5 & 5.5 \\ 3.5 & -2.5 & 1.5 & -0.5 & -7.5 & 6.5 & -5.5 & 4.5 \\ 4.5 & 5.5 & 6.5 & 7.5 & -0.5 & -1.5 & -2.5 & -3.5 \\ 5.5 & -4.5 & -7.5 & 6.5 & -1.5 & 0.5 & 3.5 & -2.5 \\ 6.5 & 7.5 & -4.5 & -5.5 & 2.5 & 3.5 & -0.5 & -1.5 \\ 7.5 & -6.5 & 5.5 & -4.5 & 3.5 & -2.5 & 1.5 & -0.5 \end{pmatrix}.$$

Based on the equality conditions of Theorem 7, we can construct H that satisfies Conditions (iv) and (v) using the Kronecker product. Let H be an $H(q, 2^q)$, it is called a Hadamard matrix if $HH^T = qI_t$. It is easy to verify that a Hadamard matrix satisfies Conditions (i), (ii) and (iii). Therefore, Proposition 2 can be obtained immediately.

Proposition 2. *Let W_1 be a U-type $H(n, 2^q)$ with $\delta(W_1) \geq q/2$ and W_2 be a Hadamard matrix $H(\lambda, 2^\lambda)$, then $W = W_1 \otimes W_2$ is an $H(\lambda n, 2^{\lambda q})$ satisfying Conditions* (iv) *and* (v).

It is well known that a saturated $OA(4\lambda, 4\lambda - 1, 2, 2)$ is Hamming equidistant with a distance of 2λ. If any one column is deleted, the resulting design must be an $OA(4\lambda, 4\lambda - 2, 2, 2)$ with a minimal pairwise Hamming distance of $2\lambda - 1$. Both of the above two designs meet Conditions (iv) and (v), thus they can be used as the U-type designs to generate designs satisfying Conditions (iv) and (v) with large sizes according to Proposition 2.

Corollary 5. *Let W_1 be a saturated $OA(4\lambda_1, 4\lambda_1-1, 2, 2)$ or an $OA(4\lambda_1, 4\lambda_1-2, 2, 2)$ by deleting one column from this saturated OA, and W_2 be a Hadamard matrix $H(\lambda_2, 2^{\lambda_2})$, then $W = (2W_1) \otimes W_2$ is an $H(4\lambda_1\lambda_2, 2^{(4\lambda_1-1)\lambda_2})$ or $H(4\lambda_1\lambda_2, 2^{(4\lambda_1-2)\lambda_2})$ satisfying Conditions* (iv) *and* (v).

The following example illustrates how to construct a design satisfying Conditions (iv) and (v) according to Corollary 5.

Example 5. Let $W_1 = \frac{1}{2}\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix}^T$ and $W_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, which are an $OA(4, 2, 2, 2)$ and a Hadamard matrix $H(2, 2^2)$, respectively. It can be verified that

$$(2W_1) \otimes W_2 = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \end{pmatrix}^T$$

is an $H(8, 2^4)$ satisfying Conditions (iv) and (v).

Theorem 8. *Let W be an $H(4\lambda_1\lambda_2, 2^{(4\lambda_1-1)\lambda_2})$ or $H(4\lambda_1\lambda_2, 2^{(4\lambda_1-2)\lambda_2})$ obtained by Corollary 5 and $G^{(k)}$ be a $D(2^k, (2^{k+1})^{2^k})$ generated by Construction 1. Then $D_0 = W \otimes G^{(k)}$ is a U-type $D(\lambda_1\lambda_2 2^{k+2}, (2^{k+1})^{(4\lambda_1-1)\lambda_2 2^k})$ or $D(\lambda_1\lambda_2 2^{k+2}, (2^{k+1})^{(4\lambda_1-2)\lambda_2 2^k})$ achieving the upper bound on the right-hand side of* (5.1).

In Theorem 8, $G^{(k)}$ satisfies Conditions (i), (ii), (iii), and W satisfies Conditions (iv) and (v). Thus, it can be verified that $d_2(W \otimes G^{(k)})$ reaches the upper bound on the right-hand side of (5.1). Example 6 shows one instance from Theorem 8.

Example 6. Let $D_0 = (2W_1) \otimes G^{(1)}$, where W_1 is shown in Example 5 and $G^{(1)} = \begin{pmatrix} 0.5 & 1.5 \\ 1.5 & -0.5 \end{pmatrix}$. Then D_0 is the U-type design D in Example 1 with $d_2(D_0) = 10$, which reaches the upper bound on the right-hand side of (5.1). According to Theorem 7, D_0 is optimal among all designs with Kronecker product structure, and we can prove that D_0 is optimal among all U-type $D(8, 4^4)$'s (See Table 2).

In fact, for a U-type $D(N, s^m)$, we have $\lfloor \bar{d}_2 \rfloor \to m(s^2-1)/6$ when $N \to \infty$. Thus, $m(s^2-1)/6$ may be the upper bound of $d_2(D)$ for all possible U-type $D(N, s^m)$'s in some situations. Similar to Theorem 2 of Wang, Yang and Xu (2018), we have the following lemma.

Lemma 3. *When $s = 4$, if m is even and $N \geq \max\{m+2, 5m/4\}$, we have $d_2(D) \leq m(s^2-1)/6$ for all U-type $D(N, s^m)$'s.*

For a $D(N, s^m)$, the distance variance criterion (Chen and Tang, 2022; Wang, Sun and Xu, 2022; Wang and Sun, 2023) is defined as $V(D) = \sum_{1\leq i<j\leq N}(d_2(\boldsymbol{x}_i, \boldsymbol{x}_j) - \bar{d}_2(D))^2$, where $\bar{d}_2(D) = 2\sum_{1\leq i<j\leq N} d_2(\boldsymbol{x}_i, \boldsymbol{x}_j)/(N(N-1))$ is the average L_2-distance between all distinct rows in D. In addition, according to Theorem 4.2 in Wang and Sun (2023), a U-type design D minimizes the value of $V(D)$ if and only if D is orthogonal and all rows are L_2-equidistant from the origin. According to the properties of $G^{(k)}$ constructed by Construction 1, we have the following proposition.

Proposition 3. *Let $D_0 = W \otimes G^{(k)}$, where W is an orthogonal U-type $H(n, 2^q)$ and $G^{(k)}$ is a $D(2^k, (2^{k+1})^{2^k})$ generated by Construction 1, then D_0 is a $D(n2^k, (2^{k+1})^{q2^k}))$, which is optimal under the distance variance criterion.*

Table 2 shows the minimal pairwise L_2-distances and the distance efficiencies of some designs obtained from Theorem 8, where, for a given $W \otimes G^{(k)}$, the value outside the parentheses is the minimal pairwise L_2-distance and the value inside the parentheses is the distance efficiency. In Table 2, W is from Corollary 5 and $G^{(k)}$ is from Construction 1. The optimality of the designs with a distance efficiency of 1 in Table 2 is derived based on Lemma 3. It is worth mentioning that all designs in Table 2 are optimal under the distance variance criterion because of the orthogonality of W.

Table 2: The minimal distances and distance efficiencies of $W \otimes G^{(k)}$ with $G^{(k)}$ being a $D(2^k, (2^{k+1})^{2^k})$.

W	$D(2, 4^2)$	$D(4, 8^4)$	$D(8, 16^8)$	$D(16, 32^{16})$
$H(4, 2^2)$	10(1)*	84(0.944)	680(0.970)	5456(0.984)
$H(4, 2^3)$	15(1)	126(0.940)	1020(0.970)	8184(0.984)
$H(8, 2^4)$	20(1)	168(0.971)	1360(0.985)	10912(0.992)
$H(8, 2^6)$	30(1)	252(0.969)	2040(0.985)	16368(0.992)
$H(8, 2^7)$	35(0.946)	294(0.970)	2380(0.985)	19096(0.992)
$H(12, 2^{10})$	50(0.962)	420(0.981)	3400(0.990)	27280(0.995)
$H(12, 2^{11})$	55(0.965)	462(0.981)	3740(0.990)	30008(0.995)
$H(16, 2^8)$	40(1)	336(0.985)	2720(0.992)	21824(0.996)
$H(16, 2^{12})$	60(1)	504(0.984)	4080(0.992)	32736(0.996)
$H(16, 2^{14})$	70(0.972)	588(0.985)	4760(0.992)	38192(0.996)
$H(16, 2^{15})$	75(0.974)	630(0.984)	5100(0.992)	40920(0.996)
$H(20, 2^{18})$	90(0.978)	756(0.988)	6120(0.994)	49104(0.997)
$H(20, 2^{19})$	95(0.979)	798(0.988)	6460(0.994)	51832(0.997)

*: "10" is the minimal pairwise L_2-distance of $H(4, 2^2) \otimes D(2, 4^2)$ and "1" inside the parentheses is the distance efficiency of $H(4, 2^2) \otimes D(2, 4^2)$. The rest are similar.

In fact, the designs obtained from Theorem 8 perform as well as some high-performance designs from the existing literature under the maximin L_2-distance criterion. Specifically, if the resulting design is a $D(N_0, s^{m_0})$, then its minimal pairwise

L_2-distance is equal to $m_0(s^2-1)/6$. Table 3 presents detailed information on the designs that can be obtained from Theorem 8 and share the same parameters as those in existing works, where N_0 denotes the run size, m_0 the number of columns, s the number of levels, D and H the corresponding designs in Theorem 8, and λ_1, λ_2 the corresponding values in Theorem 8. Here, k, k_0, and b are parameters satisfying the conditions specified in the corresponding references. Since the minimal pairwise L_2-distances of these designs are all $m_0(s^2-1)/6$, they are not included in the table.

Table 3: Details of some designs from existing works and Theorem 8.

N_0	m_0	s	D	H	λ_1	λ_2
$^{\dagger}2^{k+2}$	2^{k+1}	2^{k+2}	$G^{(k)}$	$H(2,2^1)$	/	/
$^{\ddagger}2^{k}$	$2^k-2^{k_0}$	4	$G^{(1)}$	$H(2^{k-1},2^{2^{k-1}-2^{k_0-1}})$	2^{k-k_0-2}	2^{k_0-1}
$^{\ddagger}2^{k}$	$2^k-2^{k_0}$	8	$G^{(2)}$	$H(2^{k-2},2^{2^{k-2}-2^{k_0-2}})$	2^{k-k_0-2}	2^{k_0-2}
$^{\ddagger}2^{k}$	$2^k-2^{k_0}$	16	$G^{(3)}$	$H(2^{k-3},2^{2^{k-3}-2^{k_0-3}})$	2^{k-k_0-2}	2^{k_0-3}
$^{\ddagger}2^{k}b$	$b(2^k-2^{k_0})$	4	$G^{(1)}$	$H(2^{k-1}b,2^{b(2^{k-1}-2^{k_0-1})})$	2^{k-k_0-2}	$2^{k_0-1}b$
$^{\ddagger}2^{k}b$	$b(2^k-2^{k_0})$	8	$G^{(2)}$	$H(2^{k-2}b,2^{b(2^{k-2}-2^{k_0-2})})$	2^{k-k_0-2}	$2^{k_0-2}b$
$^{\S}8$	4	4	$G^{(1)}$	$H(4,2^2)$	1	1
$^{\S}8$	6	4	$G^{(1)}$	$H(4,2^3)$	1	1
$^{\S}16$	8	4	$G^{(1)}$	$H(8,2^4)$	1	2
$^{\S}16$	14	4	$G^{(1)}$	$H(8,2^7)$	2	1
$^{\S}16$	8	8	$G^{(2)}$	$H(4,2^2)$	1	1
$^{\S}16$	12	8	$G^{(2)}$	$H(4,2^3)$	1	1
$^{\S}32$	16	8	$G^{(2)}$	$H(8,2^4)$	1	2
$^{\S}32$	28	8	$G^{(2)}$	$H(8,2^7)$	2	1

†: designs from Theorem 1 in Zhou, Yang and Liu (2020); ‡: designs from Conclusions 1–5 in Li, Tian and Liu (2024); §: designs from Table 5 in Wang and Sun (2023).

Table 3 shows that the designs obtained from Theorem 8 cover many designs from the aforementioned references, and can also generate new designs that are not listed in the table. Even for designs with identical parameters to those reported in the existing literature, we provide an alternative interpretation and construction method from the Kronecker product perspective. Our results therefore carry significant practical value.

6. Searching For Space-filling Designs

According to Theorem 1, when H is a two-level full factorial design, the value of $\phi(D_0)$ only depends on D. This also provides inspiration for our next algorithm. Let

$$\tilde{\phi}(D,q) = C(D,0,q) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{F(\boldsymbol{x}_i,\boldsymbol{x}_j)+F(\boldsymbol{x}_i,-\boldsymbol{x}_j)}{2}\right)^q$$

and H_q be a two-level full factorial design with q factors defined in Section 5. For a fixed q, we can use TA algorithm to search for the D with a small value of $\tilde{\phi}(D,q)$ and then perform a Kronecker product with H_q to obtain the final design. Algorithm 1 is used to generate space-filling designs.

In Algorithm 1, a $D(N_0, s^{m_0})$ with a small ϕ value is desired. Therefore, we should choose the appropriate N, m and q to generate it. We can set $I = 50$ and $J = 10^4$ for medium N and m. If N and m are large, $I = 100$ and $J = 10^5$ are more suitable. For τ, we can generate 1000 $D(N, s^m)$'s randomly and denote the largest and smallest $\tilde{\phi}$ values of these designs by τ_{max} and τ_{min}, respectively. Let $\tau = \alpha(\tau_{max} - \tau_{min})$, where $0 < \alpha < 1$. We can try some α's and choose the best one. For simplicity, we always choose $I = 50$, $J = 10^4$ and $\alpha = 0.1$. Actually, adding or deleting very few rows or columns has little impact on the value of ϕ. For the D_0 obtained in line 25 of Algorithm 1, we can add rows and/or columns to D_0 or delete rows and/or columns from D_0 randomly such that the final design is a $D(N_0, s^{m_0})$. If possible, we can

Algorithm 1: Kronecker threshold accepting (KTA)

input: N_0, m_0, s
Choose suitable N, m and q such that mq is close to m_0 and $N2^q$ is close to N_0
Generate a $D(N, s^m)$ randomly and denote it by D
input: I, J, τ
initialize: $i = 1$, $R = 10^{10}$ is a sufficiently large number
$D_{min} \leftarrow D$
$r_{min} \leftarrow R$
while $i \leq I$ **do**
  $j \leftarrow 1$
  while $j \leq J$ **do**
    generate D_{new} by exchanging two elements in different columns of D randomly
    if $\tilde{\phi}(D_{new}, q) < r_{min}$ **then**
      $r_{min} \leftarrow \tilde{\phi}(D_{new}, q)$
      $D_{min} \leftarrow D_{new}$
    end if
    if $\tilde{\phi}(D_{new}, q) < r_{min} + \tau$ **then**
      $D \leftarrow D_{new}$
    end if
    $j \leftarrow j + 1$
  end while
  $\tau \leftarrow (I - i)\tau/I$
  $D \leftarrow D_{min}$
  $i \leftarrow i + 1$
end while
$D_0 \leftarrow H_t \otimes D$
Add rows and/or columns to D_0 or delete rows and/or columns from D_0 such that its row size is N_0 and column size is m_0

consider as many cases as possible and choose the best one. Algorithm 1 is suitable for generating designs for which N_0 and m_0 are approximately integer multiples of 2^q

and q, respectively, for some integer q.

Compared with the original TA algorithm, we change the optimization objective function of the KTA algorithm from $\phi(D_0)$ to $\tilde{\phi}(D,q)$. The computational complexity of $\tilde{\phi}(D,q)$ is much smaller than $\phi(D_0)$ in each iteration, since their computational complexities are $O(N^2 m)$ and $O(N_0^2 m_0)$ respectively. Thus, KTA can greatly reduce the computational time.

If we choose an L_2-type discrepancy in Section 4 as the space-filling criterion, we need to make some adjustments to $\tilde{\phi}(D,q)$. For example, if we choose CD^2 and omit the constant term, let $F(\boldsymbol{x}_i,\boldsymbol{x}_j)=\prod_{k=1}^{m}(1+|x_{ik}|/(2s)+|x_{jk}|/(2s)-|x_{ik}-x_{jk}|/(2s))$, $\tilde{\phi}(D,q)$ will be adjusted to

$$\tilde{\phi}_{CD}(D,q)=-\frac{2}{N}\sum_{i=1}^{N}\prod_{k=1}^{m}\left(1+\left|\frac{x_{ik}}{2s}\right|-2\left|\frac{x_{ik}}{2s}\right|^2\right)^q+\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{F(\boldsymbol{x}_i,\boldsymbol{x}_j)+F(\boldsymbol{x}_i,-\boldsymbol{x}_j)}{2}\right)^q;$$

if we choose MD^2 and omit the constant term, let $F(\boldsymbol{x}_i,\boldsymbol{x}_j)=\prod_{k=1}^{m}(15/8-|x_{ik}|/(4s)-|x_{jk}|/(4s)-3|x_{ik}-x_{jk}|/(4s)+|x_{ik}-x_{jk}|^2/(2s^2))$, $\tilde{\phi}(D,q)$ will be adjusted to

$$\tilde{\phi}_{MD}(D,q)=-\frac{2}{N}\sum_{i=1}^{N}\prod_{k=1}^{m}\left(\frac{5}{3}-\left|\frac{x_{ik}}{4s}\right|-\left|\frac{x_{ik}}{2s}\right|^2\right)^q+\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{F(\boldsymbol{x}_i,\boldsymbol{x}_j)+F(\boldsymbol{x}_i,-\boldsymbol{x}_j)}{2}\right)^q.$$

Example 7 explains how to search for large space-filling designs by KTA when taking CD^2 as the criterion.

Example 7. We want to construct a $D(96,8^{24})$ with a small CD^2 value. All possible q values are $1,2,3,4$. To balance efficiency and time cost, $q=2$ is the most suitable choice. For $q=2$, we search for a $D(24,8^{12})$ and perform a Kronecker product with H_2 as described in KTA. Finally, we obtain a $D(96,8^{24})$ with CD$^2(D)=1.1634$. This case will also be shown in Figure 1.

We now compare the CD^2 values of different designs with medium and large sizes, the results are provided in Table S3 in the supplementary material. In that table, uniform designs (UD) are generated by the R package "UniDOE" with default parameters (Zhang et al., 2018). Existing designs (ED) are from the website http://web.stat.nankai.edu.cn/cms-ud/UD/UniformDesign.html or obtained by TA algorithm or combinatorial methods. Designs obtained by mixture method (MM) are from Zhou and Fang (2013). The bold font is the smallest one in each case. The N_0 with asterisk ($*$) means that the design has the same N_0, m_0 and s but obtained by a smaller q compared with the previous case. From Table S3, we can see that KTA performs the best or almost the best in all cases. For designs with the same N, m and s, the KTA with a smaller q performs better. The other choices of q are omitted here due to the similarity.

Figure 1 shows the CD^2 values of the designs with 24 factors and 8 levels for run sizes of 80 to 120 from different methods. It can be observed that KTA with $q = 2$ is completely superior to other methods for all run sizes and KTA with $q = 3$ also performs well. When the run size is 112 or 120, the performance of KTA with $q = 3$ is very close to that of ED and UD although it is not the best. This indicates that a smaller q can improve the performance.

Figure 2 and Table 4 further compare the CD^2 values of designs with larger sizes. When the run size increases, there is no available ED for comparison. Therefore, we only compare KTA with MM and UD respectively. Figure 2 shows the CD^2 values of the designs with 40 factors, 8 levels and run sizes of 320 to 464 obtained by KTA with

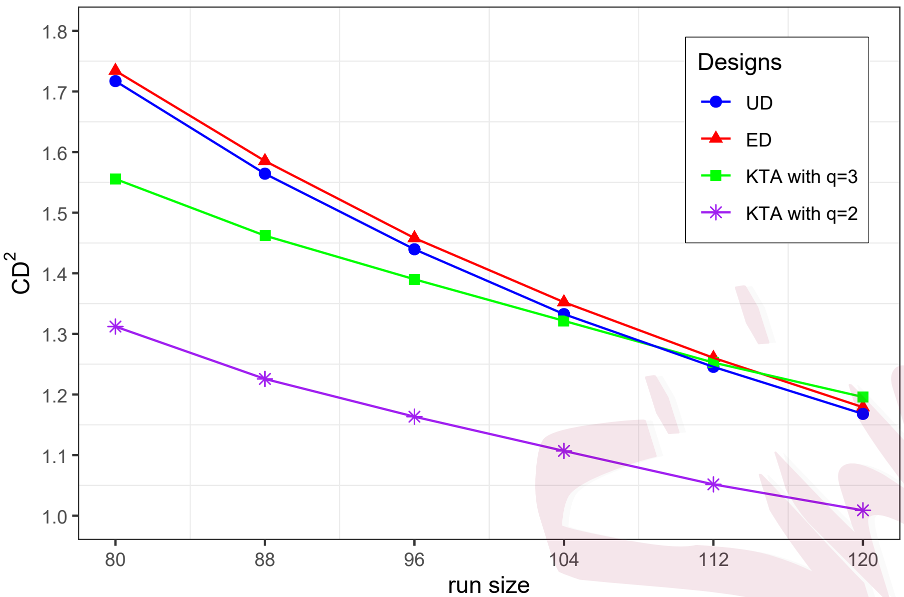

Figure 1: The CD^2 values of the designs with 24 factors and 8 levels generated by different methods.

$q = 4$ and UD. Table 4 shows the CD^2 values of the designs with different run sizes obtained by KTA and MM. When the run size becomes larger, KTA still performs better compared with MM and UD.

Table 4: The CD^2 values of different designs.

N_0	m_0	s	N	m	q	MM	KTA
215	40	5	27	13	3	13.6156	**11.6524**
301	40	5	38	13	3	11.2669	**10.3080**
311	40	5	39	13	3	11.0574	**10.1826**
401	40	4	25	10	4	12.9535	**12.0597**

In general, KTA has obvious advantages over existing methods. Even if in some cases KTA is not the best, we can choose a smaller q to improve the performance. A larger q has less computational complexity but may have worse performance compared with a smaller q due to its less search scope. So we should choose a proper q to

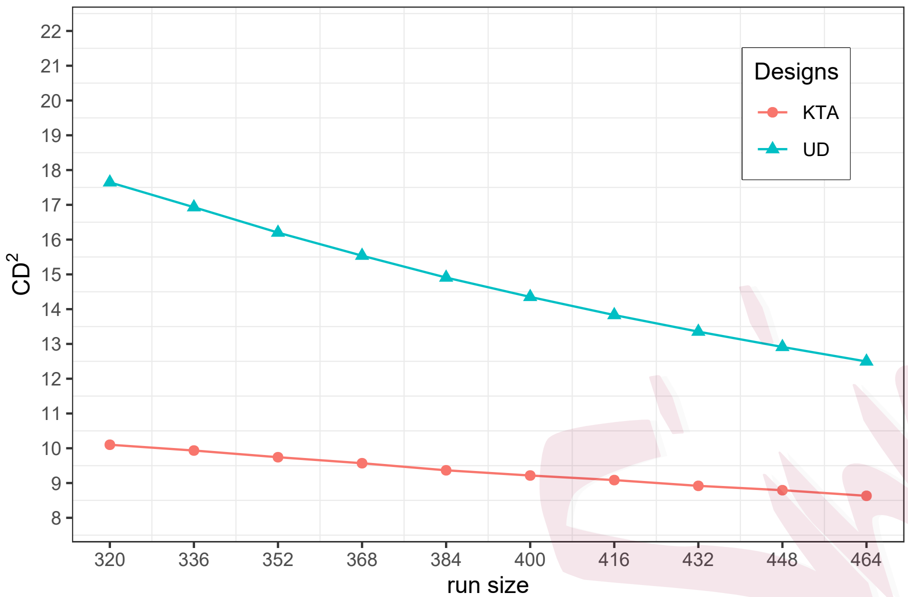

Figure 2: The CD^2 values of designs with 40 factors and 8 levels generated by KTA and UD.

balance the computational cost and performance. In the supplementary material, we present additional comparison results between the KTA algorithm and other methods under the maximum projection criterion, MD, and CD. Furthermore, we demonstrate via case studies that the design generated by the KTA algorithm exhibits excellent performance in building statistical surrogate models. These results collectively confirm the effectiveness and practical application value of the KTA algorithm.

7. Concluding Remarks

This paper discusses the relationship between various space-filling criteria and kernel functions, demonstrating that the majority of existing space-filling criteria can be expressed in terms of kernel functions. For designs with Kronecker product structure, the kernel-based space-filling criterion can be written in the form of a linear expression of the GWLP of a small two-level design, facilitating rapid computation of the criterion. Based on this linear expression, it is proved that all coefficients of the GWLP are nonnegative under some specific conditions. These results provide theoretical support for the construction of space-filling designs. Under the kernel-based space-filling criterion, we show that a U-type full design, the transposes of a COA and an OAII, are optimal among designs with the same size. Under the maximin L_2-distance criterion, construction methods of optimal designs achieving the upper bound are proposed. In addition, an algorithm is provided for generating flexible space-filling designs, demonstrating superior performance and reduced computational time compared to existing methods.

In this paper, H is restricted to a two-level design, thus imposing structural limitations on the resulting design. We may consider adopting a more general form of H in the future work. Furthermore, although we demonstrate that the lower bound in Theorem 5 can be achieved when D belongs to three special classes of designs, there may exist more designs achieving this lower bound when f is a specified kernel function. Finally, the KTA algorithm is developed for the general space-filling criterion in (2.1). When a specific space-filling criterion is employed, there might exist more suitable optimization methods. These aspects will be explored in future research.

Supplementary Material

The supplementary material discusses the corresponding results about extending the mean squared correlation criterion and distance variance criterion to (2.1) respectively, provides the proofs of some theoretical results, the additional comparisons and simulations, and a large table.

Acknowledgements

The authors thank Editor John Stufken, an associate editor and two anonymous referees for their insightful comments and suggestions. This research was supported by the National Natural Science Foundation of China (Grant Nos. 12131001, 12271270 and 12371260). The four authors are affiliated with the NITFID, LPMC, KLMDASR, and the School of Statistics and Data Science at Nankai University, and they contributed equally to this work.

References

Ai, M. Y. and Zhang, R. C. (2004). Projection justification of generalized minimum aberration for asymmetrical fractional factorial designs. *Metrika* **60**, 279–285.

Bingham, D., Sitter, R. R. and Tang, B. (2009). Orthogonal and nearly orthogonal designs for computer experiments. *Biometrika* **96**, 51–65.

Chen, G. and Tang, B. (2022). A study of orthogonal array-based designs under a broad class of space-filling criteria. *Ann. Statist.* **50**, 2925–2949.

Cheng, S. W. and Ye, K. Q. (2004). Geometric isomorphism and minimum aberration for factorial designs with quantitative factors. *Ann. Statist.* **32**, 2168–2185.

Fang, K. T., Liu, M. Q., Qin, H. and Zhou, Y. D. (2018). *Theory and Application of Uniform Experimental Designs.* Springer and Science press, Singapore and Beijing.

Hickernell, F. J. and Liu, M. Q. (2002). Uniform designs limit aliasing. *Biometrika* **89**, 893–904.

Huang, H. (2021). Construction of component orthogonal arrays with any number of components. *J. Statist. Plann. Inference* **213**, 72–79.

Johnson, M. E., Moore, L. M. and Ylvisaker, D. (1990). Minimax and maximin distance designs. *J. Statist. Plann. Inference* **26**, 131–148.

Joseph, V. R. (2016). Space-filling designs for computer experiments: A review. *Qual. Engrg.* **28**, 28–35.

Joseph, V. R., Gul, E. and Ba, S. (2015). Maximum projection designs for computer experiments. *Biometrika* **102**, 371–380.

Joseph, V. R., Gul, E. and Ba, S. (2019). Designing computer experiments with multiple types of factors: The MaxPro approach. *J. Qual. Technol.* **52**, 343–354.

Li, W., Liu, M. Q. and Tang, B. (2021). A method of constructing maximin distance designs. *Biometrika* **108**, 845–855.

Li, W., Tian, Y. and Liu, M. Q. (2024). Construction of orthogonal maximin distance designs. *J. Qual. Technol.* **56**, 312–326.

Lin, C. D., Bingham, D., Sitter, R. R. and Tang, B. (2010). A new and flexible method for constructing designs for computer experiments. *Ann. Statist.* **38**, 1460–1477.

Pang, S., Wang, J., Lin, D. K. J. and Liu, M. Q. (2021). Construction of mixed orthogonal arrays with high strength. *Ann. Statist.* **49**, 2870–2884.

Rao, C. R. (1961). Combinatorial arrangements analogous to orthogonal arrays. *Sankhya A* **23**, 283–286.

Tang, Y. and Xu, H. (2014). Permuting regular fractional factorial designs for screening quantitative factors. *Biometrika* **101**, 333–350.

Tang, Y. and Xu, H. (2021). Wordlength enumerator for fractional factorial designs. *Ann. Statist.* **49**, 255–271.

Tang, Y., Xu, H. and Lin, D. K. J. (2012). Uniform fractional factorial designs. *Ann. Statist.* **40**, 891–907.

Van Den Berg, C., Christensen, J. P. R. and Ressel, P. (2012). *Harmonic Analysis on Semigroups: Theory of Positive Definite and Related Functions.* Springer Science & Business Media, New York.

Wang, L., Xiao, Q. and Xu, H. (2018). Optimal maximin L_1-distance Latin hypercube designs based on good lattice point designs. *Ann. Statist.* **46**, 3741–3766.

Wang, Y. and Sun, F. (2023). On the maximin distance properties of orthogonal designs via the rotation. *Sci. China Math.* **66**, 1593–1608.

Wang, Y., Sun, F. and Xu, H. (2022). On design orthogonality, maximin distance, and projection uniformity for computer experiments. *J. Amer. Statist. Assoc.* **117**, 375–385.

Wang, Y., Yang, J. and Xu, H. (2018). On the connection between maximin distance designs and orthogonal designs. *Biometrika* **105**, 471–477.

Xu, H. and Wu, C. F. J. (2001). Generalized minimum aberration for asymmetrical fractional factorial designs. *Ann. Statist.* **29**, 549–560.

Yang, J. F., Sun, F. and Xu, H. (2021). A component-position model, analysis and design for order-of-addition experiments. *Technometrics* **63**, 212–224.

Zhang, A., Li, H., Quan, S. and Yang, Z. (2018). UniDOE: Uniform design of experiments. *R Package Version 1.0.2*, https://CRAN. R-project.org/package=UniDOE.

Zhao, Y., Li, Z. and Zhao, S. (2021). A new method of finding component orthogonal arrays for order-of-addition experiments. *Metrika* **84**, 805–824.

Zhou, W. P., Yang, J. F. and Liu, M. Q. (2020). Optimal maximin L_2-distance Latin hypercube designs. *J. Statist. Plann. Inference* **207**, 113–122.

Zhou, Y. D. and Fang, K. T. (2013). An efficient method for constructing uniform designs with large size. *Comput. Statist.* **28**, 1319–1331.

Zhou, Y. D. and Xu, H. (2014). Space-filling fractional factorial designs. *J. Amer. Statist. Assoc.* **109**, 1134–1144.

Zhou, Y. D. and Xu, H. (2015). Space-filling properties of good lattice point sets. *Biometrika* **102**, 959–966.