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A NEW CLASS OF ORTHOGONAL DESIGNS WITH GOOD LOW DIMENSIONAL SPACE-FILLING PROPERTIES

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Abstract: The space-filling property and orthogonality are perhaps two most desirable design properties for computer experiments. The space-filling property is appropriate for Gaussian process models, while orthogonality allows the estimated effects to be uncorrelated. This paper presents a general approach for constructing a rich class of orthogonal designs with attractive low-dimensional space-filling properties. This is apparently new in the literature. The construction methods are straightforward to implement. Their theoretical supports are established. Moreover, the resulting designs are flexible in the run sizes.

Key words and phrases: Computer experiment, orthogonal design, orthogonality, space-filling property.

1. Introduction

Computer experiments are widely used in many fields to explore complex systems; whereas space-filling designs are popular for such experiments (see, for examples, Fang, Li and Sudjianto (2006) and Santner, Williams and Note (2018)). A space-filling design uniformly spreads its points in the design region. The uniformity can be e-

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valuated by distance or discrepancy criteria (see, for examples, Johnson, Moore and Ylvisaker (1990); Fang et al. (2000); Joseph, Gul and Ba (2015) and Wang, Sun and Xu (2022)). Many fruitful approaches have been proposed for constructing designs with good space-filling properties. The Latin hypercube design was first introduced by McKay, Beckman and Conover (1979). Owen (1992) and Tang (1993) proposed randomized orthogonal arrays and orthogonal array-based Latin hypercube designs, respectively. More recently, He and Tang (2013) introduced strong orthogonal arrays, and such arrays have been further developed in He and Tang (2014), Liu and Liu (2015), He, Cheng and Tang (2018), Zhou and Tang (2019), Shi and Tang (2020), Tian and Xu (2022) and Wang, Yang and Liu (2022). Mukerjee, Sun and Tang (2014) proposed mappable nearly orthogonal arrays. Note that both strong orthogonal arrays and mappable nearly orthogonal arrays have better space-filling properties than ordinary orthogonal arrays.

Orthogonality is another desirable property for designs of computer experiments. It guarantees that the estimated effects are uncorrelated with each other. A number of methods have been proposed to construct orthogonal designs; see, for examples, Ye (1998), Steinberg and Lin (2006), Joseph and Hung (2008), Bingham, Sitter and Tang (2009), Sun, Liu and Lin (2009), Pang, Liu and Lin (2009), Lin, Mukerjee and Tang (2009), Georgiou and Stylianou (2011), Ai, He and Liu (2012), Yang and Liu (2012), Georgiou et al. (2014), Sun and Tang (2017a) and Wang et al. (2018).

This paper presents a general approach for constructing orthogonal designs that entertain attractive space-filling properties. This class of orthogonal space-filling designs is apparently new in the literature. Two appealing features of the new construction method are their simplicity and generality: the proposed method is simple as it is straightforward to implement (as will be shown below), and the method is also general in the sense that the resulting designs can be either symmetric (equal-level) or asymmetric (mixed-level). Additionally, the resulting designs are flexible in the run sizes.

The remainder of this paper is organized as follows. Section 2 introduces the notation and preliminaries. Sections 3 and 4 propose methods for constructing s^4-level and s^3-level symmetric orthogonal designs with desirable space-filling properties, respectively. Section 5 is devoted to the case of mixed-level orthogonal designs. Concluding remarks are provided in Section 6. All proofs and some tables are provided in the Supplementary Material.

2. Definitions and Preliminaries

We first review relevant terminologies and provide two lemmas for future use. Let $D(n, s_1 \times \cdots \times s_m)$ denote a mixed-level balanced design of n runs and m factors, with each of the s_i levels from $\{0, 1, \ldots, s_i - 1\}$ replicated equally often in the ith column. When all the s_j's are equal to s, the design becomes a symmetric balanced design $D(n, s^m)$. A design $D(n, s_1 \times \cdots \times s_m)$ becomes a mixed-level (combinatorial) orthogonal array of strength t and $s_1, \ldots, s_m$ levels, denoted as $\mathrm{OA}(n, m,\, s_1 \times \cdots \times s_m, t)$, if all possible level combinations for any t columns occur with the same frequency. When all the s_j's are equal to s, the array is symmetric and denoted as $\mathrm{OA}(n, m, s, t)$.

A design $D(n, p_1 \times \cdots \times p_m)$ is said to achieve a stratification on an $s_1 \times \cdots \times s_t$

grid in some t ($t \geq 2$) dimensions, say $\{i_1, \ldots, i_t\}$, if the t columns can be collapsed into an OA$(n, t, s_1 \times \cdots \times s_t, t)$, where for $k = 1, \ldots, t$, $s_k \leq p_{i_k}$ and the p_{i_k} levels of the i_kth column are collapsed into s_k levels by $\lfloor z/(p_{i_k}/s_k) \rfloor$ for $z = 0, 1, \ldots p_{i_k} - 1$, therein $\lfloor \vartheta \rfloor$ is the largest integer not exceeding ϑ. Take the following transposed array as an example

$$\begin{pmatrix} 4 & 7 & 5 & 6 & 7 & 4 & 6 & 5 & 3 & 0 & 2 & 1 & 0 & 3 & 1 & 2 \\ 0 & 6 & 5 & 3 & 7 & 1 & 2 & 4 & 7 & 1 & 2 & 4 & 0 & 6 & 5 & 3 \end{pmatrix}.$$

This array is a $D(16, 8^2)$, and can be collapsed into the following transposed OA$(16, 2, 2\times 4, 2)$

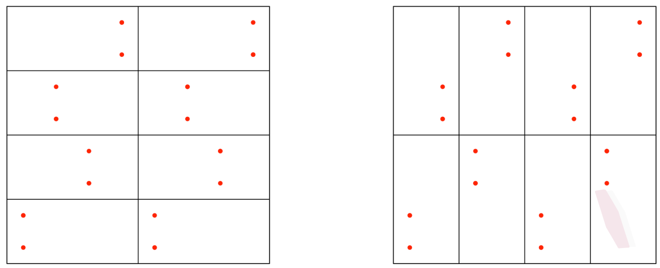
$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 2 & 1 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 0 & 3 & 2 & 1 \end{pmatrix},$$

where the 8 levels of the two factors are collapsed into two levels and four levels according to

$$\lfloor z/4 \rfloor = \begin{cases} 0, & z = 0, 1, 2, 3, \\ 1, & z = 4, 5, 6, 7, \end{cases} \text{ and } \lfloor z/2 \rfloor = \begin{cases} 0, & z = 0, 1, \\ 1, & z = 2, 3, \\ 2, & z = 4, 5, \\ 3, & z = 6, 7, \end{cases}$$

respectively. Thus the array achieves a stratification on a 2×4 grid, as shown in Figure 1 (a). Similarly, the array achieves a stratification on a 4×2 grid, as shown in Figure 1 (b).

The correlation between two centralized vectors $a = (a_1, \ldots, a_n)^T$ and $b = (b_1, \ldots, b_n)^T$ is defined as $a^T b/(\|a\|\|b\|)$, where $\|z\|$ represents the L_2 norm of vector z. A design



(a) Stratification on a 2×4 grid. (b) Stratification on a 4×2 grid.

Figure 1: Stratifications of the $D(16, 8^2)$.

$D(n, s^m)$ is said to be orthogonal, denoted as $\mathrm{OD}(n, s^m)$, if the correlation between any two columns is 0.

To facilitate the study of orthogonality, we center the s levels of design $D(n, s^m)$ into

$$\Omega(s) = \{\omega - (s-1)/2 | \omega = 0, \ldots, s-1\}. \tag{2.1}$$

The operator $*$ represents the centralization of a column, which implies that for a column d on $GF(s)$, d^* is obtained from d via the mapping in (2.1).

Let $GF(s)$ denote the Galois field of order s. For two matrices $A = (a_{ij})_{m\times n}$ and $B = (b_{ij})_{u\times v}$ with entries from $GF(s)$, their Kronecker sum is defined as

$$A \oplus B = \begin{pmatrix} a_{11} \dot{+} B & \cdots & a_{1n} \dot{+} B \\ \vdots & & \vdots \\ a_{m1} \dot{+} B & \cdots & a_{mn} \dot{+} B \end{pmatrix},$$

where $\dot{+}$ is the addition defined on $GF(s)$.

We next present two indispensable lemmas for the construction methods in the subsequent sections.

Lemma 1. *Let* $\alpha_s = (0,\ldots,s-1)^T$ *and* $\alpha_0 = (0,\ldots,0)^T$ *be two* $s \times 1$ *vectors on* $GF(s)$*.*

(i) *If* (d_1, d_2) *is an* $OA(n,2,s,2)$*, then the arrays* $(\alpha_0 \oplus d_1, \alpha_0 \oplus d_2, \alpha_s \oplus d_2)$ *and* $(\alpha_s \oplus d_1, \alpha_0 \oplus d_2, \alpha_s \oplus d_2)$ *are* $OA(sn,3,s,3)$*'s.*

(ii) *If* (d_1, d_2, d_3) *is an* $OA(n,3,s,2)$*, then the array* $(\alpha_0 \oplus d_1, \alpha_0 \oplus d_2, \alpha_s \oplus d_3)$ *is an* $OA(sn,3,s,3)$*.*

(iii) *If* (d_1, d_2, d_3) *is an* $OA(n,3,s,3)$*, then the arrays* $(\alpha_0 \oplus d_1, \alpha_0 \oplus d_2, \alpha_0 \oplus d_3, \alpha_s \oplus d_3)$*,* $(\alpha_0 \oplus d_1, \alpha_s \oplus d_2, \alpha_0 \oplus d_3, \alpha_s \oplus d_3)$ *and* $(\alpha_s \oplus d_1, \alpha_s \oplus d_2, \alpha_0 \oplus d_3, \alpha_s \oplus d_3)$ *are* $OA(sn,4,s,4)$*'s.*

Let A be an OA$(n,g,p,2)$ and B an OA$(p,m,s,2)$. In each column of A, replace the vth level by the vth row of B for $v = 1,\ldots,p$, then we get a matrix $C = (C_1,\ldots,C_g)$, where C_i represents the ith group of m columns obtained by replacing the levels in the ith column of A by the rows of B. Hedayat, Sloane and Stufken (1999) (Section 9.3) shows that C is an OA$(n,gm,s,2)$. Then we have the following lemma, which provides a basis for the proposed construction method.

Lemma 2. *Any four columns obtained by taking two columns from group* C_{i_1} *and two columns from group* C_{i_2} *with* $i_1 \neq i_2$ *must form an* $OA(n,4,s,4)$*.*

3. Orthogonal Space-filling Designs of s^4 Levels

In this section, we propose a construction method for orthogonal designs of s^4 levels and investigate their properties. The construction is given in Algorithm 1 below.

Algorithm 1 (Construction of s^4-level orthogonal designs)**.**

Input: An OA$(n, g, p, 2)$, called A, and an OA$(p, m, s, 2)$, called B.

Output: An OD$(sn, (s^4)^{4q})$ with $q = \lfloor gk/2 \rfloor$ and $k = \lfloor m/2 \rfloor$, called $\tilde{X}$.

Step 1. In each column of A, replace the vth level by the vth row of B for $v = 1, \ldots, p$, then we get a matrix

$$C = (C_1, \ldots, C_g),$$

where C_i represents the ith group of m columns obtained by replacing the levels in the ith column of A by the rows of B. For $i = 1, \ldots, g$, partition each C_i into k or $k+1$ groups as

$$C_i = (C_{i1}, \ldots, C_{ik}) \text{ if } m = 2k, \text{or } C_i = (C_{i1}, \ldots, C_{ik}, \iota_i) \text{ if } m = 2k+1,$$

where $k = \lfloor m/2 \rfloor$ and each C_{ij} consists of two columns. Note that when m is odd, the $(k+1)$th group of C_i has only one column ι_i. Here ι_i can be any column of C_i, and it will be discarded in the later construction. Then order C_{ij}'s as

$$C_{11}, C_{21}, \ldots, C_{g1}, C_{12}, C_{22}, \ldots, C_{g2}, \ldots, C_{1k}, C_{2k}, \ldots, C_{gk}.$$

Step 2. Take two successive C_{ij} at a time in the order given in Step 1, then obtain $q = \lfloor gk/2 \rfloor$ sets of four columns. Denote these sets as $C_{(1)}, \ldots, C_{(q)}$ with $C_{(l)} = (c_{(l1)}, \ldots, c_{(l4)})$, where $c_{(lr)}$ represent the rth column of $C_{(l)}$ for $l = 1, \ldots q$, $r = 1, 2, 3, 4$. Let

$$\tilde{C} = (C_{(1)}, \ldots, C_{(q)}).$$

Step 3. For $l = 1, \ldots, q$, obtain $X_{(l)}$ from $C_{(l)}$, where $X_{(l)} = (x_{(l1)}, x_{(l2)}, x_{(l3)}, x_{(l4)})$ and

$$x_{(l1)} = s^3(\alpha_0 \oplus c_{(l1)})^* + s^2(\alpha_s \oplus c_{(l2)})^* + s(\alpha_0 \oplus c_{(l2)})^* + (\alpha_0 \oplus c_{(l3)})^*,$$

$$x_{(l2)} = s^2(\alpha_s \oplus c_{(l1)})^* - s^3(\alpha_0 \oplus c_{(l2)})^* + s(\alpha_0 \oplus c_{(l1)})^* + (\alpha_0 \oplus c_{(l4)})^*,$$

$$x_{(l3)} = s^3(\alpha_0 \oplus c_{(l3)})^* + s^2(\alpha_s \oplus c_{(l4)})^* + s(\alpha_0 \oplus c_{(l4)})^* - (\alpha_0 \oplus c_{(l1)})^*,$$

$$x_{(l4)} = s^2(\alpha_s \oplus c_{(l3)})^* - s^3(\alpha_0 \oplus c_{(l4)})^* + s(\alpha_0 \oplus c_{(l3)})^* - (\alpha_0 \oplus c_{(l2)})^*,$$

therein $\alpha_0 = (0, \ldots, 0)^T$ and $\alpha_s = (0, \ldots, s-1)^T$ are two $s \times 1$ vectors on $GF(s)$, and $*$ is the centralization of the column, as given in Section 2. Combine $X_{(l)}$ by column juxtaposition, and obtain

$$\tilde{X} = (X_{(1)}, \ldots, X_{(q)}),$$

with $q = \lfloor gk/2 \rfloor$. Reorganize the $4q$ columns of $\tilde{X}$ according to the order of their leading columns in the original groups $C_1, \ldots, C_g$, and denote these new groups as $X_1, \ldots, X_g$. Further, define

$$X = (X_1, \ldots, X_g), \tag{3.1}$$

where X_i corresponds to C_i for $i = 1, \ldots, g$. Here, the order of the columns of X follows that of C while the order of the columns of $\tilde{X}$ follows that of $\tilde{C}$.

For the resulting design, we have the following theorem.

Theorem 1. *Design X obtained by Algorithm 1 is an $OD(sn, (s^4)^{4q})$, where $q = \lfloor gk/2 \rfloor$ and $k = \lfloor m/2 \rfloor$.*

From Theorem 1, the design X obtained by Algorithm 1 is an orthogonal design of s^4 levels. Moreover, this design possesses strong space-filling properties, as shown in the following theorem.

Theorem 2. *Design X obtained by Algorithm 1 has the following properties:*

(i) *any two distinct columns achieve stratifications on $s \times s^2$ and $s^2 \times s$ grids;*

(ii) *any two columns from different groups in* (3.1)*, say X_{i_1} and X_{i_2} with $i_1 \neq i_2$, achieve stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids;*

(iii) *any three distinct columns from two different groups in* (3.1)*, say X_{i_1} and X_{i_2} with $i_1 \neq i_2$, achieve a stratification on an $s \times s \times s$ grid.*

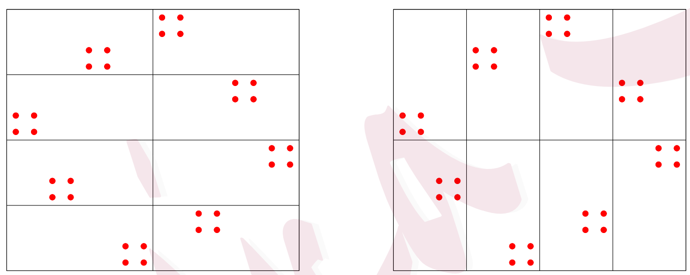
By Theorem 2, design X achieves stratifications on $s \times s^2$ and $s^2 \times s$ grids in all two dimensions, stratifications on finer $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids in those two dimensions given by two columns from different groups, and stratifications on $s \times s \times s$ grids in those three dimensions given by three columns from two different groups. Note that in X, when gk is even, there are g groups with $2k$ columns in each group; when gk is odd, there are $g-1$ groups with $2k$ columns in each group and one group of $2k-2$ columns. If $k=1$, then there are g groups with 2 columns in each group when g is even, and there are $g-1$ groups with 2 columns in each group when g is odd. If $k=2$, then gk must be even, and there are g groups with 4 columns in each group. Therefore, for $m = 2, 3, 4, 5$, the proportion of two-tuples which achieve stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids is in fact at least π with

$$\pi = (\kappa - 1)\mu/(\kappa\mu - 1), \tag{3.2}$$

if there are κ groups with μ columns in each group, where $\mu = 2k$, (i) $\kappa = g-1$ for the case of $k = 1$and odd g, and (ii) $\kappa = g$ for the other cases. An illustrative example is shown below.

Example 1. For $s = 2$, let A and B be the OA$(32, 9, 4, 2)$ and OA$(4, 3, 2, 2)$ listed in Tables S.1 and S.2 respectively in the Supplementary Material. Here $g = 9$, $k = 1$ and $q = 4$. Following Algorithm 1, we need to delete the last column of each C_i for $i = 1, \ldots, 8$. The resulting design X, an OD$(64, 16^{16})$, is shown in Table S.3 in the Supplementary Material.

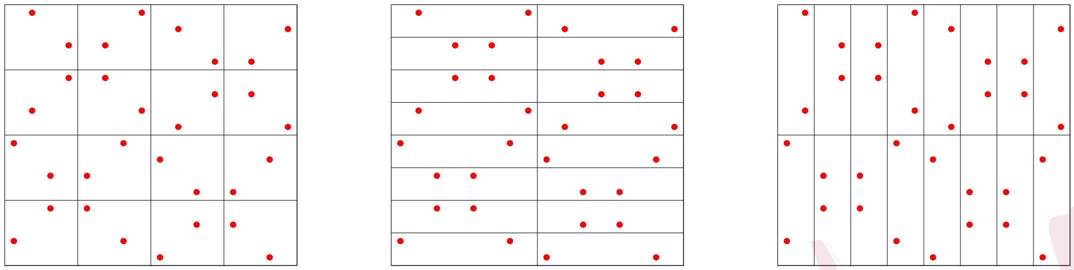
Note that X can be partitioned into eight groups with two columns in each group, such that any two columns can be respectively collapsed into an OA$(64, 2, 2 \times 4, 2)$ and an OA$(64, 2, 4 \times 2, 2)$, as displayed in Figure 2. Any two columns from different groups



(a) Stratification on a 2×4 grid. (b) Stratification on a 4×2 grid.

Figure 2: Stratifications of the first two columns of X in Example 1.

can be collapsed into an OA$(64, 2, 2 \times 8, 2)$, an OA$(64, 2, 4, 2)$ and an OA$(64, 2, 8 \times 2, 2)$, respectively, as displayed in Figure 3. Figure 4 shows the two-dimensional stratifications of the first four columns of X, where x_{ij} represents the jth column of ith group X_i. Accordingly, X achieves stratifications on 2×4 and 4×2 grids in all two dimensions, and achieves stratifications on 2×8, 4×4 and 8×2 grids in 112 out of all 120 two dimensions, thus $\pi = 93.33\%$. Further consider the three-dimensional stratification of design X. It can be checked that any three columns from two different groups achieve



(a) Stratification on a 4×4 grid. (b) Stratification on a 2×8 grid. (c) Stratification on an 8×2 grid.

Figure 3: Stratifications of the first and third columns of X in Example 1.

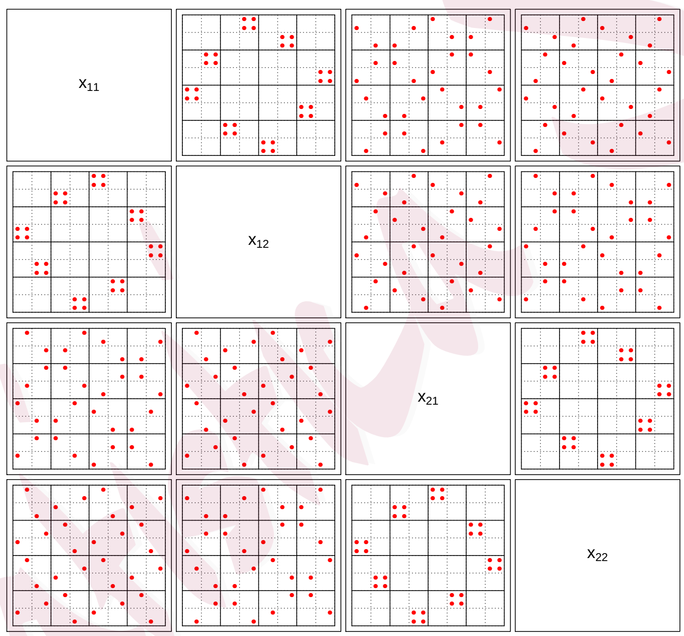


Figure 4: Two-dimensional stratifications of the first four columns of X in Example 1.

a stratification on a $2 \times 2 \times 2$ grid. In fact, the proportion of having three-tuples of X with stratifications on $2 \times 2 \times 2$ grids tends to be very high. Comprehensive examination reveals that X achieves stratifications on $2 \times 2 \times 2$ grids in 542 out of all 560 (i.e., 96.79%) three dimensions.

The orthogonal arrays needed in Algorithm 1 are available in the library of orthogonal arrays maintained by Dr. N.J.A. Sloane (http://neilsloane.com/oadir/index.html) and Hedayat, Sloane and Stufken (1999). Table 1 summarizes some orthogonal designs constructed by Algorithm 1. Their space-filling properties are characterized by the parameters κ (the number of groups), μ (the number of columns in each group) and π in (3.2). As shown in Table 1, the values of π are very close to 1, indicating that nearly all the two-tuples of these orthogonal designs achieve stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids. Moreover, these designs achieve a stratification on an $s \times s \times s$ grid in any three columns from two different groups.

Table 1: Some orthogonal designs from Algorithm 1 and their space-filling properties.

A: OA$(n, g, p, 2)$	B: OA$(p, m, s, 2)$	X: OD$(sn, (s^4)^{\kappa\mu})^\dagger$	κ	μ	$\pi(\%)$
OA$(16, 5, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(32, 16^8)$	4	2	85.71
OA$(32, 9, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(64, 16^{16})$	8	2	93.33
OA$(48, 13, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(96, 16^{24})$	12	2	95.65
OA$(64, 21, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(128, 16^{40})$	20	2	97.44
OA$(96, 23, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(192, 16^{44})$	22	2	97.67
OA$(128, 41, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(256, 16^{80})$	40	2	98.73
OA$(64, 8, 8, 2)$	OA$(8, 7, 2, 2)$	OD$(128, 16^{48})$	8	6	89.36
OA$(128, 16, 8, 2)$	OA$(8, 7, 2, 2)$	OD$(256, 16^{96})$	16	6	94.74
OA$(81, 10, 9, 2)$	OA$(9, 4, 3, 2)$	OD$(243, 81^{40})$	10	4	92.31
OA$(162, 19, 9, 2)$	OA$(9, 4, 3, 2)$	OD$(486, 81^{76})$	19	4	96.00
OA$(256, 17, 16, 2)$	OA$(16, 5, 4, 2)$	OD$(1024, 256^{68})$	17	4	95.52
OA$(512, 33, 16, 2)$	OA$(16, 5, 4, 2)$	OD$(2048, 256^{132})$	33	4	97.71
OA$(625, 26, 25, 2)$	OA$(25, 6, 5, 2)$	OD$(3125, 625^{156})$	26	6	96.77

†OD$(sn, (s^4)^{\kappa\mu})$ from Algorithm 1, which consists of κ groups of μ columns each, where $\mu = 2k$, $k = \lfloor m/2 \rfloor$, and $\kappa\mu = 4\lfloor gk/2 \rfloor$.

For comparison, we consider the resulting orthogonal designs from Algorithm 1, the mappable nearly orthogonal arrays (MNOAs) in Mukerjee, Sun and Tang (2014), the orthogonal designs in Sun and Tang (2017b), and the orthogonal strong orthogonal arrays (OSOAs) in Liu and Liu (2015). Mukerjee, Sun and Tang (2014) constructed MNOAs using a kind of replacement method (Hedayat, Sloane and Stufken (1999)), Sun and Tang (2017b) constructed orthogonal designs using rotation matrices, and Liu and Liu (2015) constructed OSOAs using generalized rotation matrices. It is worth noting that though the forms of the resulting designs are similar, the proposed method is a new technique and has not been mentioned in the literature.

By definition, an MNOA$(n, ((s^2)^u)^\phi, (s^u)^\phi)$ in Mukerjee, Sun and Tang (2014) has s^2 levels. It can be partitioned into ϕ groups with u columns in each group, where any two columns achieve a stratification on an $s \times s$ grid, and any two columns from different groups achieve a stratification on an $s^2 \times s^2$ grid. These space-filling properties also hold for the orthogonal design, denoted as OD$(n, (s^4)^m)$, in Sun and Tang (2017b), where an OD$(n, (s^4)^m)$ has s^4 levels and is orthogonal. Recall that the resulting orthogonal design from Algorithm 1 achieves stratifications on $s \times s^2$ and $s^2 \times s$ grids in all two dimensions, and stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ finer grids in any two columns from different groups. It is clear that the proposed design enjoys better two-dimensional space-filling properties compared with the MNOA$(n, ((s^2)^u)^\phi, (s^u)^\phi)$ in Mukerjee, Sun and Tang (2014) and OD$(n, (s^4)^m)$ in Sun and Tang (2017b). Moreover, it outperforms in terms of three-dimensional space-filling properties, as it achieves a stratification on an $s \times s \times s$ grid in any three dimensions from two groups.

We next consider the OSOAs in Liu and Liu (2015), denoted as OSOA$(n, m, s^3, 3)$ and OSOA$(n, m, s^4, 4)$ respectively. By the definition of strong orthogonal array (He and Tang (2013)), an OSOA$(n, m, s^3, 3)$ has s^3 levels and achieves stratifications on $s \times s^2$ and $s^2 \times s$ grids in all two dimensions, while an OSOA$(n, m, s^4, 4)$ has s^4 levels and achieves stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids in all two dimensions. It is clear that the proposed orthogonal design enjoys better one- and two-dimensional space-filling properties than the OSOA$(n, m, s^3, 3)$. It can also be regarded as a generalized version of the OSOA of strength 4, where the proportion π measures the degree of proximity in terms of two-dimensional space-filling property. From Table 1, the values of π are very close to one, i.e., the proposed designs have almost the same desirable two-dimensional space-filling properties as those of the OSOAs of strength 4. In addition, the proposed designs can accommodate much more columns.

Table 2 shows that the proposed designs enjoy much better two-dimensional space-filling properties than the MNOAs in Mukerjee, Sun and Tang (2014), orthogonal designs in Sun and Tang (2017b) and OSOAs of strength three in Liu and Liu (2015). Moreover, they have almost the same desirable two-dimensional space-filling properties as those of the OSOAs of strength 4 in Liu and Liu (2015), and they can accommodate much more columns than the latter ones. Table 3 lists the sizes of some selected designs for $s = 2$. It is clear that the proposed orthogonal designs are very competitive.

Example 2. Let $(X_i, f(X_i))$ be a computer experiment sample from the true model $f(X) = \cos(0.02\pi x_1 x_2 x_3 / x_4 - 1)$ at $X_i \in X_{\text{training}}$ for $i = 1, \ldots, 64$, where $X = (x_1, x_2, x_3, x_4)^T \in R^4$ and X_{training} is the set of training points. Fit the data by the

Table 2: Properties of the proposed orthogonal designs and related designs.

Design	Orthogonality	Stratification in two dimensions: From different groups	Stratification in two dimensions: From the same group
$\mathrm{OD}(n,(s^4)^{\kappa\mu})^{\dagger}$	1	$s\times s^3$, $s^2\times s^2$, $s^3\times s$	$s\times s^2$, $s^2\times s$
$\mathrm{MNOA}(n,((s^2)^u)^{\phi},(s^u)^{\phi})^{\ddagger}$	δ	$s^2\times s^2$	$s\times s$
$\mathrm{OD}(n,(s^4)^m)^{\sharp}$	1	$s^2\times s^2$	$s\times s$
$\mathrm{OSOA}(n,m,s^3,3)^{\flat}$	1	$s\times s^2$, $s^2\times s$	$s\times s^2$, $s^2\times s$
$\mathrm{OSOA}(n,m,s^4,4)^{\natural}$	1	$s\times s^3$, $s^2\times s^2$, $s^3\times s$	$s\times s^3$, $s^2\times s^2$, $s^3\times s$

$^{\dagger}\mathrm{OD}(n,(s^4)^{\kappa\mu}$ from Algorithm 1; $^{\ddagger}\mathrm{MNOA}(n,((s^2)^u)^{\phi},(s^u)^{\phi})$ in Mukerjee, Sun and Tang (2014), achieving orthogonality in proportion $\delta=(\phi-1)u/(\phi u-1)$; $^{\sharp}\mathrm{OD}(n,(s^4)^m)$ in Sun and Tang (2017b); $^{\flat}\mathrm{OSOA}(n,m,s^3,3)$ in Liu and Liu (2015); $^{\natural}\mathrm{OSOA}(n,m,s^4,4)$ in Liu and Liu (2015).

Table 3: Comparisons between the proposed orthogonal designs and related designs.

	$\mathrm{OD}(n,(s^4)^{\kappa\mu})^{\dagger}$		MNOA‡		$\mathrm{OD}(n,(s^4)^m)^{\sharp}$	OSOA$(3)^{\flat}$	OSOA$(4)^{\natural}$
n	$\kappa\mu$	$\pi(\%)$	$u\phi$	$\delta(\%)$	m	m	m
32	8	85.71	27	92.31	16	8	2
64	16	93.33	63	96.77	40	16	4
96	24	95.65	69	97.06	44	24	2
128	40	97.44	123	98.36	80	32	4
192	44	97.67	–	–	–	48	4
256	80	98.73	255	99.21	168	64	6

$^{\dagger}\mathrm{OD}(n,(s^4)^{\kappa\mu}$ from Algorithm 1, achieving stratifications on $s\times s^3$, $s^3\times s$ and $s^2\times s^2$ grids in proportion $\pi=(\kappa-1)\mu/(\kappa\mu-1)$; ‡MNOA: $\mathrm{MNOA}(n,((s^2)^u)^{\phi},(s^u)^{\phi})$ in Mukerjee, Sun and Tang (2014), achieving orthogonality and stratifications on $s^2\times s^2$ grids in proportion $\delta=(\phi-1)u/(\phi u-1)$; $^{\sharp}\mathrm{OD}(n,(s^4)^m)$ in Sun and Tang (2017b); $^{\flat}$OSOA(3): $\mathrm{OSOA}(n,m,s^3,3)$ in Liu and Liu (2015) $^{\natural}$OSOA(4): $\mathrm{OSOA}(n,m,s^4,4)$ in Liu and Liu (2015); Symbol – indicates that the corresponding array is not available.

second-order polynomial model

$$E(f(X)) = g(X) = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{1 \le i \le j \le 4} x_i x_j.$$

The mean squared error $MSE(g) = \sum_{X \in X_{\text{test}}} (f(X) - g(X))^2/N$ can be used to evaluate the performance of $g(X)$, where X_{test} is the set of test points and N is the cardinality of X_{test}. Take five X_{training}'s to be (1) the first four columns of the OD$(64, 16^{16})$ from Algorithm 1, (2) the MNOA$(64, (4^3)^{21}, (2^3)^{21})$ from Mukerjee, Sun and Tang (2014), (3) the OD$(64, 16^{40})$ from Sun and Tang (2017b), (4) the OSOA(64,16,8,3) from Liu and Liu (2015), and (5) the OSOA(64,4,16,4) from Liu and Liu (2015), respectively. Let X_{test} be the set of 10000 points $K \times K \times K \times K$, where $K = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$. The MSEs for the five designs can be obtained as 3.86, 5.96, 8.76, 4.64, and 0.47, respectively. It is clear that the OSOA(64,4,16,4) has the minimum MSE, as the OSOA of strength four enjoys the best space-filling properties among the five designs. The OD$(64, 16^{16})$ from Algorithm 1 produces the second smallest MSE, since it outperforms the MNOA$(64, (4^3)^{21}, (2^3)^{21})$, OD$(64, 16^{40})$, and OSOA(64,16,8,3) in terms of space-filling properties. Note that even the OSOA of strength four outperforms the newly proposed orthogonal design, it has too few columns and it will not work if X has five or more variables; while the OD$(64, 16^{16})$ always works for X having 16 or fewer variables. In summary, the proposed OD$(64, 16^{16})$ is a very competitive choice.

4. Orthogonal Space-filling Designs of s^3 Levels

Section 3 constructs orthogonal designs of s^4 levels. Another construction method is proposed which is able to increase the number of factors, while decreasing the number of levels of each factor to s^3. The detail is given in Algorithm 2 below.

Algorithm 2 (Construction of s^3-level orthogonal designs)**.**

Input: An OA$(n, g, p, 2)$, called A, and an OA$(p, m, s, 2)$, called B.

Output: An OD$(sn, (s^3)^{2gk})$ with $k = \lfloor m/2 \rfloor$, called Y.

Step 1. Let matrices C and C_{ij} be the same as in Algorithm 1. Then order C_{ij}'s as

$$C_{11}, C_{12}, \ldots, C_{1k}, C_{21}, C_{22}, \ldots, C_{2k}, \ldots, C_{g1}, C_{g2}, \ldots, C_{gk}.$$

Take one C_{ij} at a time in the order given in Step 1, then obtain gk sets of two columns each. Denote these sets as $C^{(1)}, \ldots, C^{(gk)}$ where $C^{(l)} = (c^{(l1)}, c^{(l2)})$ for $l = 1, \ldots, gk$.

Step 2. For $l = 1, \ldots, gk$, obtain $Y^{(l)}$ from $C^{(l)}$, where $Y^{(l)} = (y^{(l1)}, y^{(l2)})$ and

$$y^{(l1)} = s^2(\alpha_0 \oplus c^{(l1)})^* + s(\alpha_s \oplus c^{(l2)})^* + (\alpha_0 \oplus c^{(l2)})^*,$$

$$y^{(l2)} = s(\alpha_s \oplus c^{(l1)})^* - s^2(\alpha_0 \oplus c^{(l2)})^* + (\alpha_0 \oplus c^{(l1)})^*,$$

therein $\alpha_0 = (0, \ldots, 0)^T$ and $\alpha_s = (0, \ldots, s-1)^T$ are two $s \times 1$ vectors on $GF(s)$.

Step 3. Combine $Y^{(l)}$ by column juxtaposition to form $Y = (Y^{(1)}, \ldots, Y^{(gk)})$. Partition Y into g disjoint groups with $2k$ columns in each group, and obtain

$$Y = (Y_1, \ldots, Y_g). \tag{4.1}$$

By similar arguments for developing Theorems 1 and 2, we can prove that design Y has the following desirable properties.

Theorem 3. *Design Y obtained by Algorithm 2 is an OD$(sn, (s^3)^{2gk})$ with $k = \lfloor m/2 \rfloor$, and has the following properties:*

(i) *any two distinct columns achieve stratifications on $s \times s^2$ and $s^2 \times s$ grids;*

(ii) *any two columns from different groups in (4.1), say Y_{i_1} and Y_{i_2} with $i_1 \neq i_2$, achieve stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids;*

(iii) *any three distinct columns from two different groups in (4.1), say Y_{i_1} and Y_{i_2} with $i_1 \neq i_2$, achieve a stratification on an $s \times s \times s$ grid.*

Compared with the orthogonal designs constructed in Algorithm 1, the obtained designs from Algorithm 2 can accommodate more factors with fewer levels, while the space-filling properties in two and three dimensions are the same as those designs via Algorithm 1. An illustrative example is given below.

Example 3. Let matrices A and B be the ones used in Example 1. The resulting design Y shown in Table S.4 in the Supplementary Material has two more columns than design X in Example 1. It can be verified that Y is an OD$(64, 8^{18})$ and can be partitioned into 9 groups with two columns in each group. Any two columns of Y achieve stratifications on 2×4 and 4×2 grids, while any two columns from different groups achieve stratifications on 2×8, 4×4 and 8×2 grids. Here we have $\pi = 94.12\%$, where π is the proportion of two-tuples which achieve stratifications on 2×8, 4×4 and 8×2 grids. Any three distinct columns from two different groups achieve a stratification on a $2 \times 2 \times 2$ grid. Furthermore, Y achieves stratifications on $2 \times 2 \times 2$ grids in 788 out of all 816 (i.e., 96.57%) three dimensions by a comprehensive examination.

Table 4 lists some orthogonal designs obtained from Algorithm 2. Compared with the method in Algorithm 1, this method can increase the number of factors of the resulting design while decreasing the number of levels. Both methods produce orthogonal designs with attractive space-filling properties.

Table 4: Some orthogonal designs from Algorithm 2 and their space-filling properties.

A: OA$(n, g, p, 2)$	B: OA$(p, m, s, 2)$	X: OD$(sn, (s^3)^{\kappa\mu})^\ddagger$	κ	μ	$\pi(\%)$
OA$(16, 5, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(32, 8^{10})$	5	2	88.89
OA$(32, 9, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(64, 8^{18})$	9	2	94.12
OA$(48, 13, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(96, 8^{26})$	13	2	96.00
OA$(64, 21, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(128, 8^{42})$	21	2	97.56
OA$(96, 23, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(192, 8^{46})$	23	2	97.78
OA$(128, 41, 4, 2)$	OA$(4, 3, 2, 2)$	OD$(256, 8^{82})$	41	2	98.77
OA$(64, 9, 8, 2)$	OA$(8, 7, 2, 2)$	OD$(128, 8^{54})$	9	6	90.57
OA$(128, 17, 8, 2)$	OA$(8, 7, 2, 2)$	OD$(256, 8^{102})$	17	6	95.05
OA$(81, 10, 9, 2)$	OA$(9, 4, 3, 2)$	OD$(243, 27^{40})$	10	4	92.31
OA$(162, 19, 9, 2)$	OA$(9, 4, 3, 2)$	OD$(486, 27^{76})$	19	4	96.00
OA$(256, 17, 16, 2)$	OA$(16, 5, 4, 2)$	OD$(1024, 64^{68})$	17	4	95.52
OA$(512, 33, 16, 2)$	OA$(16, 5, 4, 2)$	OD$(2048, 64^{132})$	33	4	97.71
OA$(625, 26, 25, 2)$	OA$(25, 6, 5, 2)$	OD$(3125, 125^{156})$	26	6	96.77

‡OD$(sn, (s^3)^{\kappa\mu})$ from Algorithm 2, which consists of κ groups of μ columns each, where $\mu = 2k$, $k = \lfloor m/2 \rfloor$, and $\kappa = g$.

5. Mixed-level Orthogonal Space-filling Designs

In this section, we consider the mixed-level orthogonal designs, which are useful when some factors need more levels than others. The construction method is given in Algorithm 3.

Algorithm 3 (Construction of mixed-level orthogonal designs).

Input: An OA$(n, g, p, 2)$, called A, and an OA$(p, m, s, 2)$, called B.

Output: An OD$(sn, (s^4)^{4q_1}(s^3)^{2q_2})$ with $q_1 \leq \lfloor gk/2 \rfloor$ and $4q_1 + 2q_2 = 2gk$, called W.

Step 1. Let matrices C and C_{ij} be the same as in Algorithm 1. Then order the C_{ij}'s as

$$C_{11}, C_{21}, \ldots, C_{g1}, C_{12}, C_{22}, \ldots, C_{g2}, \ldots, C_{1k}, C_{2k}, \ldots, C_{gk}.$$

First, take two successive C_{ij}'s in the above order a total of q_1 times, where $q_1 \leq \lfloor gk/2 \rfloor$. Then we obtain q_1 sets of four columns each, denoted as $C_{(1)}, \ldots, C_{(q_1)}$, where $C_{(l)} = (c_{(l1)}, \ldots, c_{(l4)})$ for $l = 1, \ldots, q_1$. Take one C_{ij} at a time in the remaining list, then we obtain $q_2 = gk - 2q_1$ sets of two columns each, denoted as $C^{(1)}, \ldots, C^{(q_2)}$, where $C^{(l)} = (c^{(l1)}, c^{(l2)})$ for $l = 1, \ldots, q_2$.

Step 2. For $l = 1, \ldots, q_1$, let $W_{(l)}$ be the $X_{(l)}$ in Algorithm 1. For $l = 1, \ldots, q_2$, let $W^{(l)}$ be the $Y^{(l)}$ in Algorithm 2. Further let

$$\overline{W} = (W_{(1)}, \ldots, W_{(q_1)}, W^{(1)}, \ldots, W^{(q_2)}).$$

Step 3. Rearrange the columns of $\overline{W}$ according to the order of their leading columns in the original groups $C_1, \ldots, C_g$ and denote these new groups as $W_1, \ldots, W_g$. Define

$$W = (W_1, \ldots, W_g), \tag{5.1}$$

where W_i corresponds to C_i for $i = 1, \ldots, g$.

Similar to Theorem 3, we have the following theorem for the resulting design W.

Theorem 4. *Design W obtained by Algorithm 3 is an OD$(sn, (s^4)^{4q_1}(s^3)^{2q_2})$ with $q_1 \leq \lfloor gk/2 \rfloor$ and $4q_1 + 2q_2 = 2gk$, and has the following properties:*

(i) *any two distinct columns achieve stratifications on $s \times s^2$ and $s^2 \times s$ grids;*

(ii) *any two columns from different groups in (5.1), say W_{i_1} and W_{i_2} with $i_1 \neq i_2$, achieve stratifications on $s \times s^3$, $s^2 \times s^2$ and $s^3 \times s$ grids;*

(iii) *any three distinct columns from two different groups in (5.1), say W_{i_1} and W_{i_2} with $i_1 \neq i_2$, achieve a stratification on an $s \times s \times s$ grid.*

Remark 1. From Theorem 4, if gk is even and $q_1 = gk/2$, the resulting design is the OD$(sn, (s^4)^{2gk})$ obtained in Algorithm 1; if gk is odd, then for $q_1 = \lfloor gk/2 \rfloor$, we can get the OD$(sn, (s^4)^{4\lfloor gk/2 \rfloor})$ obtained in Algorithm 1 by deleting the last two columns. Taking the value of q_1 to be the minimum value 0, the design OD$(sn, (s^3)^{2gk})$ is just the one obtained via Algorithm 2.

Example 4. Let matrices A and B be the ones used in Example 1. If $q_1 = 3$, the resulting design W from Algorithm 3 is a mixed-level design with 18 columns, of which 12 factors are populated by 16 levels, and the other 6 factors are populated by 8 levels (as shown in Table S.5 in the Supplementary Material). It can be verified that this is an OD$(64, 16^{12}8^6)$ which can be partitioned into 9 disjoint groups with two columns in each group. Moreover, any two columns achieve stratifications on 2×4 and 4×2 grids, any two columns from different groups achieve stratifications on 2×8, 4×4 and 8×2 grids, and any three distinct columns from two different groups achieve a stratification on a $2 \times 2 \times 2$ grid. Furthermore, it can be verified that W achieves stratifications on

$2 \times 2 \times 2$ grids in 788 out of all 816 (i.e., 96.57%) three dimensions.

6. Concluding Remarks

The space-filling property is perhaps the most popular design property for computer experiments, as it results in good performance in terms of prediction accuracy over the entire experimental region and minimizes the bias of the fitted model. Orthogonality is also an important property for computer experiments since it allows the estimates of the main effects to be uncorrelated with each other. Therefore, both the space-filling property and orthogonality are desirable.

Here, we develop methods for constructing a new class of orthogonal designs with attractive (two- and three-dimensional) space-filling properties. These designs are new and can not be constructed by any existing methods. The resulting designs are very flexible in the run sizes —e.g., they do not necessarily need to be prime powers. These newly constructed orthogonal designs can be either symmetric (equal-level) or asymmetric (mixed-level). This is particularly useful when some factors have more levels than others. Compared with popular space-filling designs, specifically the mappable nearly orthogonal arrays in Mukerjee, Sun and Tang (2014) and orthogonal designs in Sun and Tang (2017b), the proposed designs have better space-filling properties in both two and three dimensions as well as in one dimension for s^4-level orthogonal designs from Algorithm 1.

Algorithms 1 and 2 focus on the orthogonal designs of s^4 and s^3 levels, respectively; while Algorithm 3 provides a construction for the mixed-level case of this class of orthogonal designs, which are appealing for allocating factors with different numbers of levels. Table 5 summarizes some orthogonal designs constructed by Algorithms 1, 2 and 3 for practical needs.

Table 5: Some orthogonal designs from Algorithms 1, 2 and 3.

				$\mathrm{OD}(sn,(s^4)^{4q_1}(s^3)^{2q_2})^\sharp$	
A: $\mathrm{OA}(n,g,p,2)$	B: $\mathrm{OA}(p,m,s,2)$	$\mathrm{OD}(sn,(s^4)^{4\lfloor gk/2\rfloor})^\dagger$	$\mathrm{OD}(sn,(s^3)^{2gk})^\ddagger$	Design	Constraint
$\mathrm{OA}(16,5,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(32,16^8)$	$\mathrm{OD}(32,8^{10})$	$\mathrm{OD}(32,16^{4q_1}8^{2q_2})$	$Q=10,q_1\le 2$
$\mathrm{OA}(32,9,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(64,16^{16})$	$\mathrm{OD}(64,8^{18})$	$\mathrm{OD}(64,16^{4q_1}8^{2q_2})$	$Q=18,q_1\le 4$
$\mathrm{OA}(48,13,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(96,16^{24})$	$\mathrm{OD}(96,8^{26})$	$\mathrm{OD}(96,16^{4q_1}8^{2q_2})$	$Q=26,q_1\le 6$
$\mathrm{OA}(64,21,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(128,16^{40})$	$\mathrm{OD}(128,8^{42})$	$\mathrm{OD}(128,16^{4q_1}8^{2q_2})$	$Q=42,q_1\le 10$
$\mathrm{OA}(96,23,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(192,16^{44})$	$\mathrm{OD}(192,8^{46})$	$\mathrm{OD}(192,16^{4q_1}8^{2q_2})$	$Q=46,q_1\le 11$
$\mathrm{OA}(128,41,4,2)$	$\mathrm{OA}(4,3,2,2)$	$\mathrm{OD}(256,16^{80})$	$\mathrm{OD}(256,8^{82})$	$\mathrm{OD}(256,16^{4q_1}8^{2q_2})$	$Q=82,q_1\le 20$
$\mathrm{OA}(64,9,8,2)$	$\mathrm{OA}(8,7,2,2)$	$\mathrm{OD}(128,16^{52})$	$\mathrm{OD}(128,8^{54})$	$\mathrm{OD}(128,16^{4q_1}8^{2q_2})$	$Q=54,q_1\le 13$
$\mathrm{OA}(128,17,8,2)$	$\mathrm{OA}(8,7,2,2)$	$\mathrm{OD}(256,16^{100})$	$\mathrm{OD}(256,8^{102})$	$\mathrm{OD}(256,16^{4q_1}8^{2q_2})$	$Q=102,q_1\le 25$
$\mathrm{OA}(81,10,9,2)$	$\mathrm{OA}(9,4,3,2)$	$\mathrm{OD}(243,81^{40})$	$\mathrm{OD}(243,27^{40})$	$\mathrm{OD}(243,81^{4q_1}27^{2q_2})$	$Q=40,q_1\le 10$
$\mathrm{OA}(162,19,9,2)$	$\mathrm{OA}(9,4,3,2)$	$\mathrm{OD}(486,81^{76})$	$\mathrm{OD}(486,27^{76})$	$\mathrm{OD}(486,81^{4q_1}27^{2q_2})$	$Q=76,q_1\le 19$
$\mathrm{OA}(256,17,16,2)$	$\mathrm{OA}(16,5,4,2)$	$\mathrm{OD}(1024,256^{68})$	$\mathrm{OD}(1024,64^{68})$	$\mathrm{OD}(1024,256^{4q_1}64^{2q_2})$	$Q=68,q_1\le 17$
$\mathrm{OA}(512,33,16,2)$	$\mathrm{OA}(16,5,4,2)$	$\mathrm{OD}(2048,256^{132})$	$\mathrm{OD}(2048,64^{132})$	$\mathrm{OD}(2048,256^{4q_1}64^{2q_2})$	$Q=132,q_1\le 33$
$\mathrm{OA}(625,26,25,2)$	$\mathrm{OA}(25,6,5,2)$	$\mathrm{OD}(3125,625^{156})$	$\mathrm{OD}(3125,125^{156})$	$\mathrm{OD}(3125,625^{4q_1}125^{2q_2})$	$Q=156,q_1\le 39$

‡ $\mathrm{OD}(sn,(s^4)^{4\lfloor gk/2\rfloor})$ from Algorithm 1; $^\ddagger\mathrm{OD}(sn,(s^3)^{2gk})$ from Algorithm 2; $^\sharp\mathrm{OD}(sn,(s^4)^{4q_1}(s^3)^{2q_2})$ from Algorithm 3, where $k=\lfloor m/2\rfloor$, $q_1\le\lfloor gk/2\rfloor$ and $Q=4q_1+2q_2=2gk$.

Orthogonal space-filling designs are desirable for computer experiments. The proposed designs are of great importance in both theory and practice. We hope that our work will stimulate a greater research interest in space-filling orthogonal designs.

Supplementary Material

The online Supplementary Material includes the proofs of Lemma 1 and Theorems 1 and 2, as well as five tables, where Tables S.1, S.2 and S.3 lists the $\mathrm{OA}(32,9,4,2)$, $\mathrm{OA}(4,3,2,2)$ and $\mathrm{OD}(64,16^{16})$ in Example 1, respectively. Table S.4 lists the OD(64, 8^{18}) in Example 3, and Table S.5 lists the $\mathrm{OD}(64,16^{12}8^6)$ in Example 4.

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