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Selecting strong orthogonal arrays by linear allowable level permutations

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Abstract: Space-filling designs are widely used in physical and computer experiments when the model between the response and input factors is uncertain. Recently, Chen and Tang (2022, *Ann. Statist.* 50, 2925–2949) justified the use of strong orthogonal arrays (SOAs) under a broad class of space-filling criteria. However, when allowable level permutations are applied to an SOA, a class of SOAs can be obtained with different geometrical structures and it is not clear which one should be selected for practical use. In this paper, we address this issue by considering a representative subset of allowable level permutations, called linear allowable level permutations. These special level permutations offer theoretical convenience in classifying various geometrically non-isomorphic SOAs. Based on these results, construction methods are provided to obtain SOAs that are more space-filling than those in the literature.

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1. Introduction

Space-filling designs are widely employed in various experiments to examine the relationship between a response and several input factors. The points of these designs are scattered in the design space in some uniform fashion, which renders them particularly useful when there is little prior knowledge on the true model between the response and the inputs, as is the case for computer experiments (Fang, Li and Sudjianto, 2006; Santner, Williams and Notz, 2018). For physical experiments, space-filling designs have also been developed for fractional factorial experiments where each factor has only a few levels (Zhou and Xu, 2014).

The quality of a space-filling design can be evaluated by the criteria of distance or discrepancy. Two popular such criteria are those of the maximin distance (Johnson, Moore and Ylvisaker, 1990) and the centered L_2-discrepancy (Hickernell, 1998), where the former aims at maximizing the minimum distance between the design points and the latter seeks a set of design points with uniform empirical distribution function. We refer to Wang, Xiao and Xu (2018), Sun, Wang and Xu (2019) and Li, Liu and Tang (2021) for some recent developments on these topics. Alternatively, space-filling designs can also be found among those with orthogonal columns; see Steinberg and Lin (2006), Lin et al. (2010), Georgiou et al. (2014) and Sun and Tang (2017) for the construction of these designs.

It is a common phenomenon that of all the factors under investigation, only a small portion is active and really impacts the response (Wu, 2015). Due to this factor sparsity, designs with space-filling low-dimensional projections are generally deemed preferable. One attractive class of designs of this kind are strong orthogonal arrays introduced by He and Tang (2013). These designs achieve better stratification properties in low dimensions, compared with their precursors such as Latin hypercubes (McKay, Beckman and Conover, 1979) and orthogonal array-based designs (Owen, 1992; Tang, 1993). The most economical strong orthogonal arrays in terms of run sizes are those of strength 2+ (He, Cheng and Tang, 2018). In this paper, we focus on these designs and refer to them as SOAs for convenience. For other related work in this field, we refer to Xiao and Xu (2018), Wang, Yang and Liu (2022), Tian and Xu (2022), Sun and Tang (2023) and references therein.

To study the performance of SOAs under the aforementioned space-filling criteria, Chen and Tang (2022) classified orthogonal array-based designs through allowable level permutations. When allowable level permutations are applied to columns of an SOA, the resulting designs form a class of SOAs which is space-filling on average under a broad class of space-filling criteria. However, members of this class may have different geometrical structures and it is not clear how to select a specific design for practical applications. One major challenge of this problem is that the number of allowable level permutations is often too large to handle, both theoretically and computationally.

In this paper, we address this problem by considering a subset of allowable level permutations, called linear allowable level permutations (LALPs). We show that these special level permutations are representative of all allowable ones in that the average performance of the class of resulting designs remains the same. Even more desirable is the theoretical convenience they provide for studying the structures of SOAs. Armed with LALPs, we are able to enumerate geometrically non-isomorphic patterns of SOAs and characterize those with better space-filling properties. Based on these characterization results, we provide construction methods for SOAs that are more space-filling than the existing ones in the literature.

The remainder of the paper is organized as follows. The necessary notation and background are given in Section 2. Then we introduce the concept of LALPs and study its properties in Section 3. Section 4 applies these level permutations to SOAs and presents construction methods for SOAs with better space-filling properties. Finally, the paper is concluded with a discussion in Section 5. All the proofs are postponed to the Appendix.

2. Notation and background

We represent a design D of n runs for m factors by an $n \times m$ matrix. For $j = 1, \ldots, m$, the entries of the jth column are from the integer ring $\mathbb{Z}_{s_j} = \{0, 1, \ldots, s_j - 1\}$ if the jth factor has s_j levels. The design D is said to be an orthogonal array of strength t and denoted by $\mathrm{OA}(n, s_1 \times \cdots \times s_m, t)$ if any t columns of D contain all possible level combinations equally often. If $s_1 = \cdots = s_m = s$, we also denote the array by $\mathrm{OA}(n, m, s, t)$. An $\mathrm{OA}(s^k, m, s, t)$ is regular if it can be constructed by first writing down k independent columns, and then adding $m-k$ interaction columns thereof. We refer to Hedayat, Sloane and Stufken (1999) for a comprehensive account on orthogonal arrays.

In this paper, we study space-filling designs based on orthogonal arrays. An $\mathrm{OA}(n, m, s^2, 1)$ is said to be an orthogonal array-based design, and denoted by $\mathrm{OABD}_s(n, (s^2)^m)$ if it can be collapsed into an $\mathrm{OA}(n, m, s, 2)$, where collapsing s^2 levels into s levels is done by $\lfloor x/s \rfloor$ for $x = 0, 1, \ldots, s^2$. An $\mathrm{OABD}_s(n, (s^2)^m)$ is called a strong orthogonal array of strength 2+ (SOA) and denoted by $\mathrm{SOA}_s(n, (s^2)^m)$ if any two of its columns can be collapsed into an $\mathrm{OA}(n, s^2 \times s, 2)$ as well as an $\mathrm{OA}(n, s \times s^2, 2)$. In other words, any two-dimensional projection of an $\mathrm{OABD}_s(n, (s^2)^m)$ is stratified over an $s \times s$ grid while that of an $\mathrm{SOA}_s(n, (s^2)^m)$ achieves stratification over finer $s^2 \times s$ and $s \times s^2$ grids. It is therefore appropriate to say that $\mathrm{SOA}_s(n, (s^2)^m)$'s are superior members in the whole class of $\mathrm{OABD}_s(n, (s^2)^m)$'s. Both $\mathrm{OABD}_s(n, (s^2)^m)$'s and $\mathrm{SOA}_s(n, (s^2)^m)$'s can be characterized in terms of two component arrays A and B as follows (He, Cheng and Tang, 2018).

Lemma 2.1. *Design D is an $\mathrm{OABD}_s(n, (s^2)^m)$ if and only if there exist $A = (a_1, \ldots, a_m)$ and $B = (b_1, \ldots, b_m)$ such that $D = sA + B$ where A is an $\mathrm{OA}(n, m, s, 2)$ and (a_j, b_j) is an $\mathrm{OA}(n, 2, s, 2)$ for $j = 1, \ldots, m$. Furthermore, D is an $\mathrm{SOA}_s(n, (s^2)^m)$ if and only if (a_i, a_j, b_j) is an $\mathrm{OA}(n, 3, s, 3)$ for all $i \neq j$.*

A permutation σ on $\mathbb{Z}_{s^2}$ is s-allowable if for two levels $x, y \in \mathbb{Z}_{s^2}$, we have $\lfloor x/s \rfloor = \lfloor y/s \rfloor$ if and only if $\lfloor \sigma(x)/s \rfloor = \lfloor \sigma(y)/s \rfloor$. Therefore there are $(s!)^{s+1}$ s-allowable level permutations for $\mathbb{Z}_{s^2}$ in total. Chen and Tang (2022) showed that the stratification properties of $\mathrm{OABD}_s(n, (s^2)^m)$'s and $\mathrm{SOA}_s(n, (s^2)^m)$'s are preserved if s-allowable level permutations are applied to the columns of these designs. This we summarize as a lemma.

Lemma 2.2. *Suppose that D is an $\mathrm{OA}(n, m, s^2, 1)$ and D' is obtained by applying s-allowable level permutations to columns of D independently. Then D is an $\mathrm{OABD}_s(n, (s^2)^m)$ if and only if D' is an $\mathrm{OABD}_s(n, (s^2)^m)$; D is an $\mathrm{SOA}_s(n, (s^2)^m)$ if and only if D' is an $\mathrm{SOA}_s(n, (s^2)^m)$.*

Remark 1. Tian and Xu (2022) introduced general strong orthogonal arrays (GSOAs). According to their definition, an $\mathrm{OABD}_s(n, (s^2)^m)$ is a GSOA of strength 2.

Remark 2. More formally, the stratification properties of an $\mathrm{OA}(n, m, s^2, 1)$ can be evaluated by a space-filling pattern introduced by Tian and Xu (2022).

It can be verified that the space-filling pattern of such a design is invariant under s-allowable level permutations.

3. Linear allowable level permutations

According to Lemma 2.2, a class of $\text{OABD}_s(n,(s^2)^m)$'s can be obtained by applying s-allowable level permutations to columns of a specific $\text{OABD}_s(n,(s^2)^m)$. Despite all of them possessing the same stratification properties, designs within this class are not equally space-filling. To select a design for practical use, a brute force search is computationally unwieldy since the number of s-allowable level permutations is too large even for moderate s. For example, there are 1296 3-allowable level permutations for $\mathbb{Z}_9$ and over 2.9×10^{12} 5-allowable level permutations for $\mathbb{Z}_{25}$. To meet this challenge, we introduce a subset of allowable level permutations called linear allowable level permutations.

In the remainder of the paper, we assume that s is a prime number and thus $\mathbb{Z}_s$ is a finite field of order s. Note that any element x of $\mathbb{Z}_{s^2}$ can be written as $x = sx_a + x_b$, where $x_a = \lfloor x/s\rfloor$ and $x_b = x - s\lfloor x/s\rfloor$.

Definition 3.1. A permutation σ on $\mathbb{Z}_{s^2}$ is called a linear allowable level permutation (LALP) if for $x = sx_a + x_b \in \mathbb{Z}_{s^2}$, we have $\sigma(x) = sx'_a + x'_b$ where $x'_a = \alpha_0 + \alpha_1 x_a \pmod s$ and $x'_b = \beta_0 + \beta_1 x_a + \beta_2 x_b \pmod s$ for some $\alpha_0, \beta_0, \beta_1 \in \mathbb{Z}_s$ and some $\alpha_1, \beta_2 \in \mathbb{Z}_s \setminus \{0\}$.

It can easily be verified by definition that any LALP on $\mathbb{Z}_{s^2}$, as its name suggests, is indeed an s-allowable level permutation. The next lemma shows that all such level permutations as a whole enjoy some useful balanced properties.

Lemma 3.2. *Suppose $x, y \in \mathbb{Z}_{s^2}$. Then when σ ranges over all LALPs on $\mathbb{Z}_{s^2}$, $(\sigma(x),\sigma(y))$ contains any pair $(\hat{x},\hat{y})$ satisfying $\hat{x}\neq\hat{y}$ and $\lfloor\hat{x}/s\rfloor = \lfloor\hat{y}/s\rfloor$ exactly $s(s-1)$ times if $x\neq y$ and $\lfloor x/s\rfloor = \lfloor y/s\rfloor$, and contains any pair $(\hat{x},\hat{y})$ satisfying $\lfloor\hat{x}/s\rfloor \neq \lfloor\hat{y}/s\rfloor$ exactly $s-1$ times if $\lfloor x/s\rfloor \neq \lfloor y/s\rfloor$.*

By Definition 3.1, a linear level permutation is determined by five parameters α_0, α_1, β_0, β_1 and β_2. Hence there are $s^3(s-1)^2$ LALPs for $\mathbb{Z}_{s^2}$ in total. For $\mathbb{Z}_4$, all the 2-allowable level permutations are LALPs. The two notions of level permutations are different for $s > 2$, as illustrated in Example 1.

Example 1. Among the 1296 3-allowable level permutations of $\mathbb{Z}_9$, only $3^3\times 2^2 = 108$ of them are LALPs. For instance, $(8,7,6,4,3,5,0,2,1)$ is an LALP but $(8,7,6,4,3,5,2,1,0)$ is not, where each vector represents a permutation σ by $(\sigma(0),\ldots,\sigma(8))$.

We now study the two-dimensional projections of a design with LALPs. Suppose $D = (x_{ij})_{n\times 2}$ is a design of n runs for 2 factors. Then the commonly-used space-filling criteria such as those of maximin distance, centered L_2-discrepancy and orthogonality can all be written in a general form as

$$q(D) = \gamma_0 + \frac{\gamma_1}{n}\sum_{i=1}^{n} g(x_{i1})g(x_{i2}) + \frac{\gamma_2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} f(x_{i1},x_{j1})f(x_{i2},x_{j2}) \qquad (1)$$

for some real constants γ_0, γ_1 and $\gamma_2 > 0$ and some real functions f and g. For example, if we take $\gamma_0 = \gamma_1 = 0$, $\gamma_2 = 1$ and $f(x, y) = r^{d(x,y)}$, where $d(x, y)$ is the distance between levels x and y, then, according to Zhou and Xu (2014), the criterion $q(D) = \sum_{i=1}^{n}\sum_{j=1}^{n} r^{d_{ij}}/n^2$ extends the maximin distance criterion when $r > 0$ is sufficiently small, where $d_{ij} = d(x_{i1}, x_{j1}) + d(x_{i2}, x_{j2})$ is the distance between the ith and jth runs of D. In particular, minimizing $q(D)$ is equivalent to a criterion that sequentially minimizes $B_0(D), B_1(D), \ldots$, where $B_l(D)$ is the number of pairs of runs with distance equal to l. This criterion is a refinement of the maximin distance criterion whereas the variance of distances used in Chen and Tang (2022) is just a surrogate for the maximin distance criterion.

Chen and Tang (2022) proved that when all allowable level permutations are applied to columns of an orthogonal array-based design, the average performance in terms of q is determined by two types of stratification properties. Thanks to the balanced properties described in Lemma 3.2, the same result can also be established for LALPs. Some notation is necessary to state the result. Divide the s^2 levels of $\mathbb{Z}_{s^2}$ into s groups as $\mathbb{Z}_{s^2} = \cup_{l=0}^{s-1} S_l$, where $S_l = \{sl, sl+1, \ldots, sl+s-1\}$ for $l = 0, \ldots, s-1$. Then let $X_f = \sum_{x=0}^{s-1} f(x, x)/s$, $Y_f = \sum_{l=0}^{s-1}\sum_{x,y\in S_l, x\neq y} f(x, y)/(s^2(s-1))$ and $Z_f = \sum_{0\leq k\neq l\leq s-1}\sum_{x\in S_k, y\in S_l} f(x, y)/(s^3(s-1))$, respectively, calculate the average f-value of two levels that are the same, are distinct but from the same groups, and are from different groups. Let A_i be the number of generalized words of length i for $i = 2$ and 3 (Xu and Wu, 2001).

Theorem 3.3. *Suppose $D = sA + B$ is an $\text{OABD}_s(n, (s^2)^2)$, where $A = (a_1, a_2)$ and $B = (b_1, b_2)$. Let $\bar{q}(D)$ be the average of $q(D')$ s over all designs D' obtained by conducting LALPs to columns of D. Then*

$$\bar{q}(D) = \frac{\gamma_2}{s^4}(Y_f - X_f)^2 A_2(D) + \frac{\gamma_2}{s^3}(Y_f - X_f)(Z_f - Y_f)\mu(D) + C, \qquad (2)$$

where $\mu(D) = A_2(a_1, b_2) + A_2(a_2, b_1) + A_3(a_1, a_2, b_1) + A_3(a_1, a_2, b_2)$ and C is a constant.

Theorem 3.3 indicates that when LALPs are applied, the average performance of the all resulting designs is the same as that under all allowable level permutations. In this sense, the set of LALPs are representative of all allowable ones.

Some intuition can be acquired as to why the LALPs are representative by introducing a distance between level permutations. Let σ_1 and σ_2 be two level permutations on $\mathbb{Z}_{s^2}$ and define the distance between them as $d(\sigma_1, \sigma_2) = \sum_{x\in\mathbb{Z}_{s^2}} |\sigma_1(x) - \sigma_2(x)|$. If we apply σ_1 and σ_2 to a design, then intuitively, the two resulting designs will have similar space-filling properties if $d(\sigma_1, \sigma_2)$ is small. It is easy to come up with two allowable level permutations with a distance of 2. For $\mathbb{Z}_9$, it can be checked that the minimum distance between any two of the 108 LALPs is 6. Moreover, the distance from any nonlinear 3-allowable level permutation to its nearest LALP is either 2 or 4. For $\mathbb{Z}_{25}$, the minimum distance of two LALPs is 30.

As discussed in Chen and Tang (2022), superiority of SOAs within the whole class of orthogonal array-based designs is also reflected in their achieving small $\bar{q}(D)$ values by making $\mu(D) = 0$. In the next section, we investigate how to find regular SOAs with even better space-filling properties, through the use of LALPs.

4. Regular strong orthogonal arrays

4.1. Geometrically non-isomorphic patterns

An SOA, say $D = sA+B$, is said to be regular if columns of A and B are selected from a regular orthogonal array. Most SOAs studied in the literature are regular (He, Cheng and Tang, 2018; Shi and Tang, 2020; Zhou and Tang, 2019). The aim of this section is to enhance the space-filling properties of regular SOAs by LALPs. Unless otherwise specified, all SOAs considered in the remainder of the paper are obtained by applying LALPs to columns of regular SOAs. Lemma 4.1 gives all possible two-dimensional projections of such arrays.

Lemma 4.1. *Suppose $D = sA + B$ is an $\mathrm{SOA}_s(s^k, (s^2)^2)$. Then D is either an $\mathrm{OA}(s^k, 2, s^2, 2)$ or a design with $A = (\alpha_{10} + \alpha_{11}e_1, \alpha_{20} + \alpha_{21}e_2)$ and $B = (\beta_{10}+\beta_{11}e_1+\beta_{12}e_3, \beta_{20}+\beta_{21}e_2+\beta_{22}e_3)$ for some $\alpha_{10}, \alpha_{20}, \beta_{10}, \beta_{11}, \beta_{20}, \beta_{21} \in \mathbb{Z}_s$ and $\alpha_{11}, \alpha_{21}, \beta_{12}, \beta_{22} \in \mathbb{Z}_s \setminus \{0\}$, where e_1, e_2 and e_3 are independent columns.*

According to Cheng and Ye (2004), two designs are said to be geometrically isomorphic if they can be obtained from each other by permuting columns and/or reversing the level order in one or more columns. Geometrically isomorphic designs have the same space-filling properties. Lemma 4.1 enables us to enumerate geometrically non-isomorphic two-dimensional projections of an SOA. Through a computer search, we find that for any $k \geq 3$, there are 4 geometrically non-isomorphic $\mathrm{SOA}_2(2^k, 4^2)$'s in all, which are displayed in Fig. 1, and 12 geometrically non-isomorphic $\mathrm{SOA}_3(3^k, 9^2)$'s in all, which are displayed in Fig. 2.

For $k \geq 4$, each point in the panels of Fig. 1 and Fig. 2 is replicated s^k/s^3 times, which may be undesirable for computer experiments. One can remove the replicated points by expanding the s^2 levels to s^k levels in the same way as constructing orthogonal array-based Latin hypercubes in Tang (1993). The resulting designs will inherit the stratification properties of the original designs. Then every point in these patterns represents a stratum as seen from an $s^2 \times s^2$ grid.

Notably, some patterns in Fig. 1 and Fig. 2 are more space-filling than others. In Table 1, the 12 non-isomorphic $\mathrm{SOA}_3(3^k, 9^2)$ patterns are compared under the criteria of minimum L_1-distance between strata (Distance), the centered L_2-discrepancy (CD $\times 10^3$) and the squared correlation coefficient (Orthogonality), from which it can be seen that our intuition is in line with that reflected by the distance criterion: for some patterns the minimum L_1-distance between any two strata is 2, while for others it is only 1. The next theorem characterizes this distance feature using Lemma 4.1.

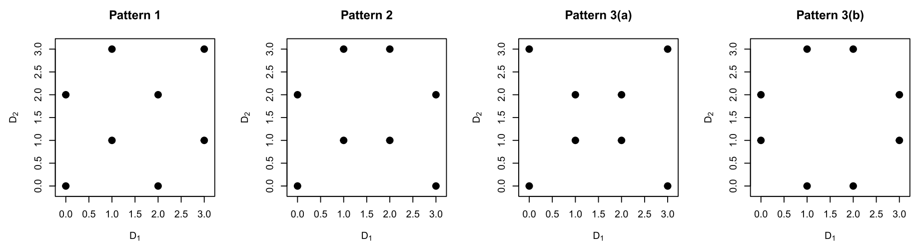

FIG 1. *Patterns of geometrically non-isomorphic* $\mathrm{SOA}_2(2^k, 4^2)$*'s.*

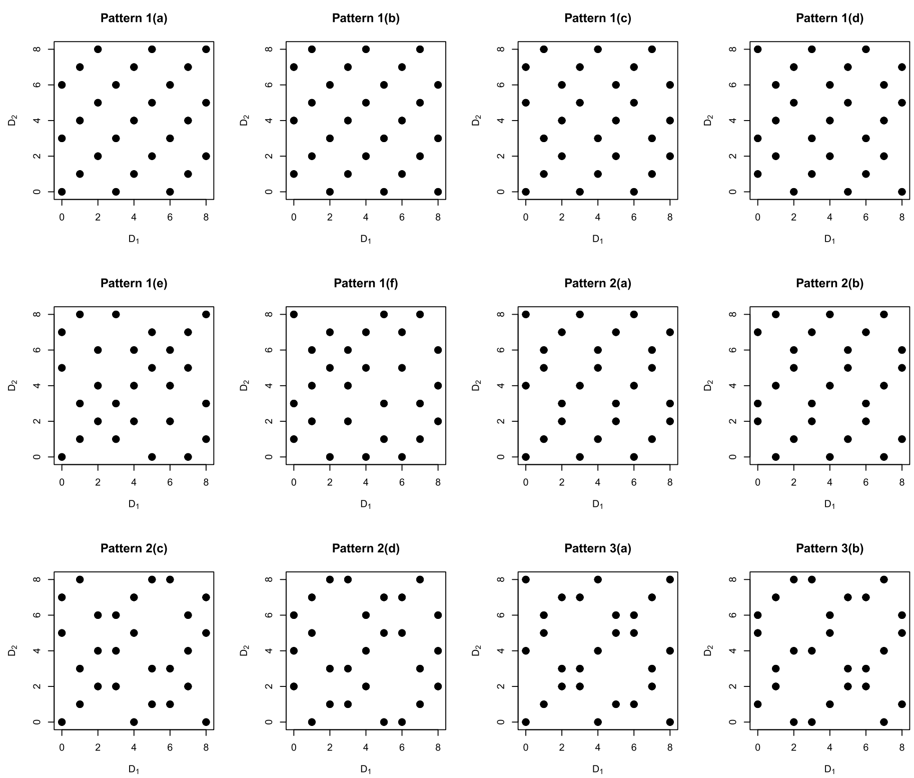

FIG 2. *Patterns of geometrically non-isomorphic* $\mathrm{SOA}_3(3^k, 9^2)$*'s.*

Theorem 4.2. *Suppose* $D = sA + B$ *is an* $\mathrm{SOA}_s(s^k, (s^2)^2)$ *with* $A = (\alpha_{10} + \alpha_{11}e_1, \alpha_{20} + \alpha_{21}e_2)$ *and* $B = (\beta_{10} + \beta_{11}e_1 + \beta_{12}e_3, \beta_{20} + \beta_{21}e_2 + \beta_{22}e_3)$ *for some independent columns* e_1*,* e_2 *and* e_3*. Let* d_{min} *be the minimum* L_1*-distance between any two strata. Then we have:*

(i) If $\alpha_{11} \neq \beta_{11}$ *and* $\alpha_{21} \neq \beta_{21}$*, then* $d_{min} > 1$*.*

(ii) If exactly one of $\alpha_{11} = \beta_{11}$ *and* $\alpha_{21} = \beta_{21}$ *holds, then* $d_{min} = 1$ *and there are* $s(s-1)$ *pairs of strata achieving* d_{min}*.*

TABLE 1
Space-filling measures of the 12 nonisomorphic $\mathrm{SOA}_3(3^k, 9^2)$*'s in Fig. 2*

Pattern	1(a)	1(b)	1(c)	1(d)	1(e)	1(f)	2(a)	2(b)	2(c)	2(d)	3(a)	3(b)
Distance	2	2	2	2	2	2	1	1	1	1	1	1
CD $\times 10^3$	2.40	2.35	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36
Orthogonality	0.1^2	0.05^2	0	0	0	0	0	0	0	0	0	0

(iii) If $\alpha_{11} = \beta_{11}$ *and* $\alpha_{21} = \beta_{21}$*, then* $d_{min} = 1$ *and there are* $2s(s-1)$ *pairs of strata achieving* d_{min}*.*

Theorem 4.2 shows that if an $\mathrm{SOA}_s(s^k, (s^2)^2)$ is not an $\mathrm{OA}(s^k, 2, s^2, 2)$, then it must be one of the three types: (i) the distance of any two strata is greater than 1, as shown in Pattern 1 of Fig. 1 and Patterns 1(a) to 1(f) of Fig. 2; (ii) there are $s(s-1)$ pairs of strata with distance 1, as shown in Pattern 2 of Fig. 1 and Patterns 2(a) to 2(d) of Fig. 2; and (iii) there are $2s(s-1)$ pairs of strata with distance 1, as shown in Patterns 3(a) and 3(b) of Fig. 1 and Fig. 2. Obviously, we prefer type (i) over type (ii) and type (ii) over type (iii).

We conclude this subsection with a remark on the relationship between level permutations and geometrically non-isomorphic patterns.

Remark 3. While there are 12 patterns of $\mathrm{SOA}_3(3^k, 9^2)$'s obtained from LALPs, there are 1017 geometrically non-isomorphic $\mathrm{SOA}_3(3^k, 9^2)$'s when all 3-allowable level permutations are considered. Among these 1017 patterns, 805 of them have $d_{min} = 1$ and 212 of them have $d_{min} = 2$. Hence, the 12 $\mathrm{SOA}_3(3^k, 9^2)$'s from LALPs do include designs with the best performance under the maximin distance criterion. This demonstrates the usefulness of LALPs in reducing the complexity of the problem.

4.2. Construction results

For an SOA, it is desirable to eliminate the two-dimensional projections of type (iii), type (ii) and type (i) sequentially. Given an $\mathrm{SOA}_s(s^k, (s^2)^m)$, say D, let $F_1(D)$, $F_2(D)$ and $F_3(D)$ be the frequencies of two-dimensional projections that are of type (i), type (ii) and type (iii), respectively. Then clearly, $F_1(D) = F_2(D) = F_3(D) = 0$ if and only if D is an $\mathrm{OA}(s^k, m, s^2, 2)$, which exists only when $m \leq (s^k - 1)/(s^2 - 1)$.

The next best things to an $\mathrm{OA}(s^k, m, s^2, 2)$ are $\mathrm{SOA}_s(s^k, (s^2)^m)$'s with $F_2(D) = F_3(D) = 0$. We now present a construction method for such designs. Suppose $e_1, \ldots, e_k$ are the k independent columns of a saturated regular $\mathrm{OA}(s^k, (s^k - 1)/(s-1), s, 2)$ where $k \geq 3$. Let $A = (a_1, \ldots, a_m)$ where $m = (s^{k-1} - 1)/(s-1)$ collect $e_1, \ldots, e_{k-1}$ and all their possible interaction columns. Let $B = (b_1, \ldots, b_m)$ where $b_i = \beta_i a_i + e_k \pmod{s}$ for $i = 1, \ldots, m$. Then we have the following result on $D = sA + B$.

Theorem 4.3. *The design* D *constructed above is an* $\mathrm{SOA}_s(s^k, (s^2)^m)$ *with* $F_2(D) = F_3(D) = 0$ *if* $\beta_i \neq 1$ *for* $i = 1, \ldots, m$*. Furthermore, the number of factors* $m = (s^{k-1} - 1)/(s-1)$ *reaches the maximum value when* $s = 2$*.*

The design D in Theorem 4.3 can also be regarded as obtained by applying LALPs to a column-orthogonal strong orthogonal array constructed in Zhou and Tang (2019). A design is said to be column-orthogonal if the correlation coefficient of any two columns is exactly zero. However, before level permutation, all the two-dimensional projections of their designs are of type (iii), and are isomorphic to Pattern 3(a) of Fig. 1 for $s = 2$ and to Pattern 3(a) of Fig. 2 for $s = 3$. After level permutation, all the two-dimensional projections are of type (i). We illustrate this construction method by Example 2.

Example 2. For $s = 5$ and $k = 3$, choose $\beta_i = 2$ for $i = 1, \cdots, 6$ and then let $A = (e_1, e_2, e_1 + e_2, e_1 + 2e_2, e_1 + 3e_2, e_1 + 4e_2) \pmod 5$ and $B = (2e_1 + e_3, 2e_2 + e_3, 2e_1 + 2e_2 + e_3, 2e_1 + 4e_2 + e_3, 2e_1 + e_2 + e_3, 2e_1 + 3e_2 + e_3) \pmod 5$. Then $D = 5A + B$ is an $\text{SOA}_5(125, (25)^6)$ with $F_2(D) = F_3(D) = 0$.

Remark 4. While all the two-dimensional projections are of type (i) so long as $\beta_i \neq 1$ for $i = 1, \ldots, m$, different choices of β_i's may lead to different type (i) patterns. For example, for $s = 3$ and $k = 3$, $(3e_1 + b_1, 3e_2 + b_2)$ with $b_i = \beta_i e_i + e_3 \pmod 3$ for $i = 1, 2$ will be isomorphic to Pattern 1(a) of Fig. 2 if $\beta_1 = \beta_2 = 0$, to Pattern 1(c) if $\beta_1 = 0$ and $\beta_2 = 2$, and to Pattern 1(e) if $\beta_1 = \beta_2 = 2$. Exactly how the coefficients β_i's are related to various type (i) patterns for general $s \geq 3$ is an interesting problem that deserves further investigation, especially if certain type (i) patterns are deemed more preferable than others. In this paper, we focus on the elimination of patterns of types (ii) and (iii), as they are clearly worse than those of type (i).

Remark 5. As noted by Zhou and Tang (2019), one can replace a_i by $a_i + e_k \pmod 2$ when $s = 2$. The resulting design achieves additional $2 \times 2 \times 2$ stratification in all three-dimensions.

The SOA given in Theorem 4.3 requires that the number m of factors be no greater than $(s^{k-1} - 1)/(s - 1)$. A recursive construction can be utilized to obtain SOAs with more factors. Suppose $D = sA + B$ is an $\text{SOA}_s(s^k, (s^2)^m)$. Let e_1 and e_2 be two independent columns of $\text{OA}(s^{k+2}, (s^{k+2} - 1)/(s - 1), s, 2)$ that do not occur in $\text{OA}(s^k, (s^k - 1)/(s - 1), s, 2)$. For $s = 2$, let

$$\tilde{A} = (A, e_1 + A, e_2 + A, e_1 + e_2 + A, e_1 + e_2),$$
$$\tilde{B} = (B, e_1 + e_2 + B, e_1 + B, e_2 + B, e_1) \pmod 2.$$

For $s \geq 3$, let

$$\tilde{A} = (\tilde{A}_{0,0}, \ldots, \tilde{A}_{s-1,s-1}, e_1), \quad \tilde{B} = (\tilde{B}_{0,0}, \ldots, \tilde{B}_{s-1,s-1}, e_2) \pmod s, \tag{3}$$

where $\tilde{A}_{\alpha,\beta} = \alpha e_1 + \beta e_2 + A$, $\tilde{B}_{\alpha,\beta} = \beta v e_1 + \alpha e_2 + B$ for $\alpha, \beta \in \mathbb{Z}_s$ and $v \in \mathbb{Z}_s$ is such that $v \neq u^2$ for any $u \in \mathbb{Z}_s$. Then we have the following result on $\tilde{D} = s\tilde{A} + \tilde{B}$.

Theorem 4.4. *Design $\tilde{D}$ is an $\text{SOA}_s(s^{k+2}, (s^2)^{ms^2+1})$ with $F_i(\tilde{D}) = s^2 F_i(D)$ for $i = 1, 2, 3$.*

We note that $A_2(D)$ is proportional to $\sum_{i=1}^{3} F_i(D)$, and thus we have $A_2(\tilde{D}) = s^2 A_2(D)$. Chen and Tang (2022) noticed this property for $s = 2$ and 3, and use these special cases to obtain strong orthogonal arrays with small A_2 values. The construction presented in Theorem 4.4 is more general as it works for any prime number of levels. More importantly, we show that $F_i(\tilde{D})$ is completely determined by $F_i(D)$ and thus the construction is useful for generating large designs with small F_2 and F_3 values.

Remark 6. The element v used in the construction is known as a quadratic nonresidue in $\mathbb{Z}_s$. As shown in Theorem A.23 in Hedayat, Sloane and Stufken (1999), there are $(s-1)/2$ such elements in $\mathbb{Z}_s$ for any odd prime s.

The small designs to be used in Theorem 4.4 can be obtained via a computer search. Suppose $D = sA + B$ is a regular $\text{SOA}_s(s^k, (s^2)^m)$, where $A = (a_1, \ldots, a_m)$ and $B = (b_1, \ldots, b_m)$. To sequentially minimize F_3, F_2 and F_1 by LALPs, Theorem 4.2 indicates only s special level permutations need to be considered for the ith column of D, and are given by replacing b_i by $\beta_i a_i + b_i$ (mod s) where $\beta_i \in \mathbb{Z}_s$ for $i = 1, \ldots, m$. Therefore, there are a total of s^m permuted designs from an initial $\text{SOA}_s(s^k, (s^2)^m)$. Nonetheless, there are still too many $\text{SOA}_s(s^k, (s^2)^m)$'s that can be used as initial designs. Hence, we restrict ourselves to SOAs with small A_2 values. According to Theorem 3.3, these designs are attractive under a broad class of space-filling criteria. In addition, since A_2 is proportional to $\sum_{i=1}^{3} F_i$, these designs tend to have small F_i values for $i = 1, 2, 3$ as well. Chen and Tang (2022) tabulated some $\text{SOA}_2(16, 4^m)$'s, $\text{SOA}_2(32, 4^m)$'s, $\text{SOA}_3(27, 9^m)$'s and $\text{SOA}_3(81, 9^m)$'s with small A_2 values; all these designs are available online at `https://github.com/gz-chen/SOA`. Starting from these designs, we apply LALPs to sequentially minimize F_3, F_2 and F_1 values. All the permuted designs are evaluated if s^m is less than 10 million, otherwise we randomly select 10 million designs and document the best one. The (F_3, F_2, F_1)'s of the obtained designs are displayed in Table 2. The detailed constructions of these designs are available upon request.

We note that by Theorem 4.3, we can construct designs with $F_3(D) = F_2(D) = 0$ when $m \leq (s^{k-1} - 1)/(s - 1)$. The designs presented in Table 2 may have nonzero $F_2(D)$ entries for these cases, but they have smaller A_2 values and thus a higher proportion of projections that are $\text{OA}(s^k, 2, s^2, 2)$. We conclude this section with an illustration of Theorem 4.4.

Example 3. Table 2 records an $\text{SOA}_3(81, 9^{13})$, say $D = 3A + B$, with $F_3(D) = 0$, $F_2(D) = 5$ and $F_1(D) = 7$. Note that the only quadratic nonresidue of $\mathbb{Z}_3$ is $v = 2$. Let $\tilde{A}_{\alpha,\beta} = \alpha e_1 + \beta e_2 + A$ and $\tilde{B}_{\alpha,\beta} = \beta v e_1 + \alpha e_2 + B$. Then $\tilde{D} = 3\tilde{A} + \tilde{B}$, where $\tilde{A}$ and $\tilde{B}$ are given in (3), is an $\text{SOA}_3(729, 9^{118})$ with $F_3(\tilde{D}) = 0$, $F_2(\tilde{D}) = 45$ and $F_1(\tilde{D}) = 63$. Moreover, by the results of Chen and Tang (2022), this design also has the minimum A_2 value among all $\text{SOA}_3(729, 9^{118})$'s.

TABLE 2
The $(F_3(D), F_2(D), F_1(D))$'s of the $\mathrm{SOA}_s(s^k, (s^2)^m)$*'s before and after LALPs*

		$(F_3(D), F_2(D), F_1(D))$				$(F_3(D), F_2(D), F_1(D))$	
s	$s^k \times m$	Before LALPs	After LALPs	s	$s^k \times m$	Before LALPs	After LALPs
2	16×6	$(1, 1, 1)$	$(0, 0, 3)$	3	27×5	$(2, 4, 4)$	$(0, 4, 6)$
2	16×7	$(1, 4, 1)$	$(0, 5, 1)$	3	27×6	$(2, 7, 6)$	$(0, 9, 6)$
2	16×8	$(2, 8, 2)$	$(1, 8, 3)$	3	81×11	$(0, 1, 3)$	$(0, 0, 4)$
2	16×9	$(3, 12, 3)$	$(3, 12, 3)$	3	81×12	$(1, 3, 4)$	$(0, 0, 8)$
2	16×10	$(8, 14, 8)$	$(5, 20, 5)$	3	81×13	$(1, 5, 6)$	$(0, 5, 7)$
2	32×10	$(0, 1, 0)$	$(0, 0, 1)$	3	81×14	$(4, 5, 7)$	$(0, 6, 10)$
2	32×11	$(0, 1, 2)$	$(0, 0, 3)$	3	81×15	$(3, 9, 9)$	$(0, 10, 11)$
2	32×12	$(2, 3, 0)$	$(0, 3, 2)$	3	81×16	$(3, 13, 11)$	$(0, 13, 14)$
2	32×13	$(2, 5, 1)$	$(0, 5, 3)$	3	81×17	$(8, 11, 15)$	$(0, 17, 17)$
2	32×14	$(2, 7, 2)$	$(0, 9, 2)$	3	81×18	$(5, 17, 20)$	$(0, 24, 18)$
2	32×15	$(5, 4, 5)$	$(0, 13, 1)$	3	81×19	$(8, 21, 22)$	$(0, 32, 19)$
2	32×16	$(4, 11, 4)$	$(1, 16, 2)$	3	81×20	$(11, 21, 31)$	$(1, 36, 26)$
2	32×17	$(7, 12, 7)$	$(3, 17, 6)$	3	81×21	$(16, 18, 41)$	$(2, 44, 29)$
2	32×18	$(8, 18, 7)$	$(5, 22, 6)$	3	81×22	$(12, 33, 50)$	$(4, 47, 44)$
2	32×19	$(10, 25, 8)$	$(7, 28, 8)$	3	81×23	$(13, 46, 58)$	$(6, 52, 59)$
2	32×20	$(12, 29, 13)$	$(9, 34, 11)$	3	81×24	$(20, 58, 64)$	$(8, 60, 74)$
2	32×21	$(18, 31, 23)$	$(12, 42, 18)$	3	81×25	$(19, 70, 76)$	$(10, 70, 85)$
2	32×22	$(27, 44, 27)$	$(18, 50, 30)$				

5. Discussion

Strong orthogonal arrays enjoy attractive stratification properties in low dimensions. Under allowable level permutations, the stratification properties of SOAs are preserved but the geometrical structure may be altered. In this paper, we select a space-filling SOA among those obtained by linear allowable level permutations (LALPs). The LALPs not only are representative but also offer convenience in characterizing various two-dimensional patterns. We then provide construction methods for more space-filling SOAs based on the characterization results.

Section 4 selects SOAs based on the maximin L_1-distance criterion. When polynomial models are considered appropriate, SOAs with orthogonal columns may also be desirable. Propositions 5.1 and 5.2 below show how such SOAs can be obtained from LALPs.

Proposition 5.1. *The design D in Theorem 4.3 has orthogonal columns as long as $\beta_i \neq 0$ for $i = 1, \ldots, m$.*

As a construction method, Proposition 5.1 itself is not surprising, since the design D in Theorem 4.3 can be viewed as obtained from the column-orthogonal SOA in Zhou and Tang (2019). What makes the result interesting is that combining with Theorem 4.3, we are able to obtain an SOA which enjoys both the properties of $F_2(D) = F_3(D) = 0$ and column orthogonality by choosing $\beta_i \neq 0, 1$ for $i = 1, \ldots, m$. For instance, the $\mathrm{SOA}_5(125, (25)^6)$ obtained in Example 2 has orthogonal columns in addition to $F_2(D) = F_3(D) = 0$.

With the aid of LALPs, we can further establish a relationship between column orthogonality and the property of $F_3(D) = 0$. Suppose $A = (a_1, \ldots, a_m)$ and $B = (b_1, \ldots, b_m)$ are such that $D = sA + B$ is an $\mathrm{SOA}_s(s^k, (s^2)^m)$. For

$i = 1, \ldots, m$, let $b'_i = (s-1)a_i + b_i \pmod{s}$ and $B' = (b'_1, \ldots, b'_m)$. Then we have the following result on D and $D' = sA + B'$.

Proposition 5.2. *We have $F_3(D) = 0$ if and only if B' is an* $\mathrm{OA}(s^k, m, s, 2)$ *and D' is a column orthogonal $SOA_s(s^k, (s^2)^m)$.*

According to Proposition 5.2, a column-orthogonal $\mathrm{SOA}_s(s^k, (s^2)^m)$ is immediately available from an $\mathrm{SOA}_s(s^k, (s^2)^m)$ with $F_3(D) = 0$. For example, the $\mathrm{SOA}_3(81, 9^{19})$ shown in Table 2 has $F_3(D) = 0$ after LALPs and hence a column-orthogonal $\mathrm{SOA}_3(81, 9^{19})$ can be obtained. Using the recursive construction in Theorem 4.4, we can obtain an $\mathrm{SOA}_3(729, 9^{172})$ with $F_3(\tilde{D}) = 0$ and thus a column-orthogonal $\mathrm{SOA}_3(729, 9^{172})$. In comparison, the method of Zhou and Tang (2019) can only yield column-orthogonal $\mathrm{SOA}_3(81, 9^{13})$ and $\mathrm{SOA}_3(729, 9^{121})$ for the corresponding run sizes.

Some directions are open for future research. In this paper, we focus on the case where the number of levels is the square of a prime number s. The concept of LALPs can also be extended to the case of s being a prime power by making use of the Galois field. A Galois field $\mathrm{GF}(s)$ is a finite field with s elements equipped with operations of addition and multiplication, and exists for any prime power s. Let ϕ be a bijection from $\mathrm{GF}(s)$ to $\mathbb{Z}_s$. Then a LALP σ on $\mathbb{Z}_{s^2}$ can be defined as one such that for $x = sx_a + x_b \in \mathbb{Z}_{s^2}$, we have $\sigma(x) = sx'_a + x'_b$ where $x'_a = \phi(\alpha_0 + \alpha_1\phi^{-1}(x_a))$ and $x'_b = \phi(\beta_0 + \beta_1\phi^{-1}(x_a) + \beta_2\phi^{-1}(x_b))$ for some $\alpha_0, \beta_0, \beta_1 \in \mathrm{GF}(s)$ and some $\alpha_1, \beta_1 \in \mathrm{GF}(s) \setminus \{0\}$. It can be verified that the results of Lemma 3.2 and Theorem 3.3 still hold for LALPs defined as above. However, the characterization result in Theorem 4.2 may no longer be valid. It is of practical interest to examine how to select more space-filling SOAs in this situation.

We apply LALPs to regular SOAs in this paper and thus the run sizes of the designs obtained are prime powers. If more flexible run sizes are needed, one could consider using LALPs to general orthogonal array-based designs. A complete enumeration of two-dimensional patterns may be difficult in this situation since the base designs are nonregular, but LALPs should still provide some computational convenience due to their representativeness.

This paper concentrates on strong orthogonal arrays of strength two plus and their two-dimensional projections. If more resources are available, we could consider the use of strong orthogonal arrays of higher strengths. Suppose $D = (x_{ij})_{n\times l}$ is an l-dimensional projection of a design. Then similar to (1), the space-filling measures such as those of maximin distance and centered L_2-discrepancy can be written as

$$q(D) = \gamma_0 + \frac{\gamma_1}{n}\sum_{i=1}^{n}\prod_{k=1}^{l} g(x_{ik}) + \frac{\gamma_2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{l} f(x_{ik}, x_{jk}) \tag{4}$$

for some real constants γ_0, γ_1 and $\gamma_2 > 0$ and real functions f and g. Following similar arguments to those in the proof of Theorem 3.3, one can show that in terms of $q(\cdot)$ in (4), the average performance of resulting designs obtained from all allowable level permutations is the same as that obtained from LALPs.

Therefore, it would be interesting to study higher-dimensional projections of SOAs with higher strengths under LALPs and find those that are most space-filling.

Appendix: proofs

Proof of Lemma 3.2. Write $x = sx_a + x_b$ and $y = sy_a + y_b$ with $0 \le x_b, y_b \le s-1$. Similarly, write $\hat{x} = s\hat{x}_a + \hat{x}_b$ and $\hat{y} = s\hat{y}_a + \hat{y}_b$ with $0 \le \hat{x}_b, \hat{y}_b \le s-1$. By Definition 3.1, applying a LALP σ to x and y gives $\sigma(x) = sx'_a + x'_b$ and $\sigma(y) = sy'_a + y'_b$, where $x'_a = \alpha_0 + \alpha_1 x_a$, $x'_b = \beta_0 + \beta_1 x_a + \beta_2 x_b$, $y'_a = \alpha_0 + \alpha_1 y_a$ and $y'_b = \beta_0 + \beta_1 y_a + \beta_2 y_b$.

(i). If $x \ne y$ and $\lfloor x/s \rfloor = \lfloor y/s \rfloor$, then we have $x_a = y_a$ and $x_b \ne y_b$. Similarly, $\hat{x} \ne \hat{y}$ and $\lfloor \hat{x}/s \rfloor = \lfloor \hat{y}/s \rfloor$ imply that $\hat{x}_a = \hat{y}_a$ and $\hat{x}_b \ne \hat{y}_b$. It can be easily seen that for each $\alpha_1 \in \mathbb{Z}_s \setminus \{0\}$, there exists a unique $\alpha_0 \in \mathbb{Z}_s$ such that $x'_a = \hat{x}_a$ and $y'_a = \hat{y}_a$. On the other hand, we have $x_b - y_b \ne 0$ due to $x_b \ne y_b$. Since $\mathbb{Z}_s \setminus \{0\}$ forms a multiplicative group, we know that there must exist a unique $\beta_2 \in \mathbb{Z}_s \setminus \{0\}$ such that $\beta_2(x_b - y_b) = \hat{x}_b - \hat{y}_b$. With this β_2, it is clear that for each $\beta_1 \in \mathbb{Z}_s$, there exists a unique $\beta_0 \in \mathbb{Z}_s$ such that $x'_b = \hat{x}_b$ and $y'_b = \hat{y}_b$. Therefore, there are a total of $s(s-1)$ choices of $(\alpha_0, \alpha_1, \beta_0, \beta_1, \beta_2)$ such that $\sigma(x) = \hat{x}$ and $\sigma(y) = \hat{y}$.

(ii). If $\lfloor x/s \rfloor \ne \lfloor y/s \rfloor$, then we have $x_a \ne y_a$. Similarly, $\lfloor \hat{x}/s \rfloor \ne \lfloor \hat{y}/s \rfloor$ implies $\hat{x}_a \ne \hat{y}_a$. Then there exists a unique $\alpha_1 \in \mathbb{Z}_s \setminus \{0\}$ such that $\alpha_1(x_a - y_a) = \hat{x}_a - \hat{y}_a$. With this α_1, there exists a unique $\alpha_0 \in \mathbb{Z}_s$ such that $x'_a = \hat{x}_a$ and $y'_a = \hat{y}_a$. Note that $x_a \ne y_a$. It can be shown with similar arguments that for each $\beta_2 \in \mathbb{Z}_s \setminus \{0\}$, there exists a unique $\beta_0 \in \mathbb{Z}_s$ and a unique $\beta_1 \in \mathbb{Z}_s$ such that $x'_b = \hat{x}_b$ and $y'_b = \hat{y}_b$. As a result, there are $s-1$ choices of $(\alpha_0, \alpha_1, \beta_0, \beta_1, \beta_2)$ such that $\sigma(x) = \hat{x}$ and $\sigma(y) = \hat{y}$. This completes the proof. □

Proof of Theorem 3.3. Let $\mathcal{D}$ be the set of all D' s obtained by applying LALPs to columns of D and $|\mathcal{D}|$ be its cardinality. Also denote the ith row of D' by (x'_{i1}, x'_{i2}). Then we have

$$\bar{q}(D) = \frac{1}{|\mathcal{D}|} \sum_{D' \in \mathcal{D}} \left\{ \gamma_0 + \frac{\gamma_1}{n} \sum_{i=1}^{n} g(x'_{i1}) g(x'_{i2}) + \frac{\gamma_2}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} f(x'_{i1}, x'_{j1}) f(x'_{i2}, x'_{j2}) \right\}$$
$$= \gamma_0 + \gamma_1 \left\{ \frac{1}{s} \sum_{x=0}^{s-1} g(x) \right\}^2 + \frac{\gamma_2}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ \frac{1}{|\mathcal{D}|} \sum_{D' \in \mathcal{D}} f(x'_{i1}, x'_{j1}) f(x'_{i2}, x'_{j2}) \right\}.$$

If $x_{i1} = x_{j1}$, then $x'_{i1} = x'_{j1}$ and we have $\sum_{D' \in \mathcal{D}} f(x'_{i1}, x'_{j1})/|\mathcal{D}| = X_f$. If $\lfloor x_{i1}/s \rfloor = \lfloor x_{j1}/s \rfloor$ and $x_{i1} \ne x_{j1}$, then $\lfloor x'_{i1}/s \rfloor = \lfloor x'_{j1}/s \rfloor$ and $x'_{i1} \ne x'_{j1}$, and by results of Lemma 3.2 we have $\sum_{D' \in \mathcal{D}} f(x'_{i1}, x'_{j1})/|\mathcal{D}| = Y_f$. Similarly, if $\lfloor x_{i1}/s \rfloor \ne \lfloor x_{j1}/s \rfloor$ then $\lfloor x'_{i1}/s \rfloor \ne \lfloor x'_{j1}/s \rfloor$ and by Lemma 3.2 we have $\sum_{D' \in \mathcal{D}} f(x'_{i1}, x'_{j1})/|\mathcal{D}| = Z_f$. Hence we have

$$\bar{q}(D) = \gamma_0 + \gamma_1 \left\{ \frac{1}{s} \sum_{x=0}^{s-1} g(x) \right\}^2 + \frac{\gamma_2}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} X_f^{\delta_{ij}(D)} Y_f^{\delta_{ij}(\lfloor D/s \rfloor) - \delta_{ij}(D)} Z_f^{2 - \delta_{ij}(\lfloor D/s \rfloor)},$$

where $\delta_{ij}(\lfloor D/s \rfloor)$ and $\delta_{ij}(D)$ are the number of coincidences between the ith and jth runs of $\lfloor D/s \rfloor = (\lfloor x_{ij}/s \rfloor)$ and D respectively. The remainder of the proof is similar to that of Theorem 2 of Chen and Tang (2022). □

Proof of Lemma 4.1. Suppose that $D_0 = sA_0 + B_0$ is a regular $\text{SOA}_s(s^k, (s^2)^2)$, where $A_0 = (a_{10}, a_{20})$ and $B_0 = (b_{10}, b_{20})$. Since A_0 and B_0 are regular, their columns can be seen as points in the projective geometry $PG(k-1, s)$. Consider two lines $L_1 = (a_{10}, b_{10}, a_{10} + b_{10}, \ldots, a_{10} + (s-1)b_{10})$ and $L_2 = (a_{20}, b_{20}, a_{20} + b_{20}, \ldots, a_{20} + (s-1)b_{20})$ in $PG(k-1, s)$. Then there are two possibilities for L_1 and L_2: (i) L_1 and L_2 do not intersect; (ii) L_1 and L_2 intersect at one point. In case (i), D_0 forms an $\text{OA}(s^k, 2, s^2, 2)$ and level permutations do not affect this combinatorial orthogonality. In case (ii), let e_3 be the intersection point, $e_1 = a_{10}$ and $e_2 = a_{20}$. Then e_1, e_2, e_3 must be independent columns since (a_{10}, a_{20}, e_3) has strength 3. Applying LALPs to columns of D_0 gives rise to D with A and B as specified in Lemma 4.1. □

Proof of Theorem 4.2. Consider two distinct points $p^{(1)} = (p_1^{(1)}, p_2^{(1)})$ and $p^{(2)} = (p_1^{(2)}, p_2^{(2)})$ of D, where

$$\begin{aligned} p_1^{(1)} &= s(\alpha_{10} + \alpha_{11}x_1) + (\beta_{10} + \beta_{11}x_1 + \beta_{12}z_1), \\ p_2^{(1)} &= s(\alpha_{20} + \alpha_{21}y_1) + (\beta_{20} + \beta_{21}y_1 + \beta_{22}z_1), \\ p_1^{(2)} &= s(\alpha_{10} + \alpha_{11}x_2) + (\beta_{10} + \beta_{11}x_2 + \beta_{12}z_2), \\ p_2^{(2)} &= s(\alpha_{20} + \alpha_{21}y_2) + (\beta_{20} + \beta_{21}y_2 + \beta_{22}z_2). \end{aligned}$$

Note that all operations within brackets are modulo s. If $p_1^{(1)} \neq p_1^{(2)}$ and $p_2^{(1)} \neq p_2^{(2)}$, then the distance between $p^{(1)}$ and $p^{(2)}$ must be greater than 1. Consider the case $p_1^{(1)} = p_1^{(2)}$ and thus $x_1 = x_2 = x$, $z_1 = z_2 = z$. Then $y_1 \neq y_2$ since $p^{(1)}$ and $p^{(2)}$ are distinct. Let $y_1' = \alpha_{20} + \alpha_{21}y_1 \pmod{s}$ and $y_2' = \alpha_{20} + \alpha_{21}y_2 \pmod{s}$. If $y_1' - y_2' \neq \pm 1$, then the distance between $p^{(1)}$ and $p^{(2)}$ must be greater than 1. Suppose $y_2' = y_1' + 1$. Then the distance between $p^{(1)}$ and $p^{(2)}$ equals to 1 if and only if

$$\begin{cases} \beta_{20} + \beta_{21}y_1 + \beta_{22}z = s - 1 \pmod{s}, \\ \beta_{20} + \beta_{21}y_2 + \beta_{22}z = 0 \pmod{s}. \end{cases} \tag{5}$$

Note that $y_2' = y_1' + 1$ implies that $\alpha_{20} + \alpha_{21}y_1 \neq 0 \pmod{s}$ and that $y_2 = y_1 + \alpha_{21}^{-1}$. Combining this with (5), we conclude that the distance between $p^{(1)}$ and $p^{(2)}$ equals to 1 if and only if $\alpha_{21} = \beta_{21}$. In addition, since x can take any element of $\mathbb{Z}_s$ and y_1 can take any element such that $\alpha_{20} + \alpha_{21}y_1 \neq 0 \pmod{s}$, there are a total of $s(s-1)$ such pairs of points. The same arguments also apply to $p_1^{(1)}$ and $p_1^{(2)}$. Therefore, if both $\alpha_{11} = \beta_{11}$ and $\alpha_{21} = \beta_{21}$, there will be $2s(s-1)$ pairs of points with distance being 1. If $\alpha_{11} \neq \beta_{11}$ and $\alpha_{21} \neq \beta_{21}$, then any pair of points would have distance greater than 1. This completes the proof. □

Proof of Theorem 4.3. Clearly, any two-dimensional projection of D is in the form given in Theorem 4.2 and satisfy the condition in part (i) of the theorem. Therefore, we have $d_{min} > 1$ and $F_2(D) = F_3(D) = 0$. Next, we show that if $D = sA + B$ is an $\text{SOA}_2(2^k, 4^m)$ with $F_2(D) = F_3(D) = 0$ then we must have $m \leq 2^{k-1} - 1$. Suppose $A = (a_1, \ldots, a_m)$ and $B = (b_1, \ldots, b_m)$. Then according to Theorem 4.2, $(a_1, \ldots, a_m, a_1 + b_1, \ldots, a_m + b_m) \pmod 2$ must be an $\text{OA}(2^k, 2m, 2, 2)$. Thus $2m \leq 2^k - 1$, from which we conclude $m \leq 2^{k-1} - 1$. □

Proof of Theorem 4.4. The proof for $s = 2$ can be done by a direct verification. Consider the case $s \geq 3$. For $u \in \mathbb{Z}_s$, let $u\tilde{A} + \tilde{B} = (u\tilde{A}_{0,0} + \tilde{B}_{0,0}, \ldots, u\tilde{A}_{s-1,s-1} + \tilde{B}_{s-1,s-1}, ue_1 + e_2)$. Note that $u\tilde{A}_{\alpha,\beta} + \tilde{B}_{\alpha,\beta} = (\alpha u + \beta v)e_1 + (\beta u + \alpha)e_2 + uA + B$. Since $v \neq u^2$ for any $u \in \mathbb{Z}_s$, there exists a unique solution (α, β) to

$$\begin{cases} \alpha u + \beta v = \alpha' \pmod s, \\ \beta u + \alpha = \beta' \pmod s \end{cases}$$

for any $\alpha' \in \mathbb{Z}_s$ and $\beta' \in \mathbb{Z}_s$. The fact that this holds for any $u \in \mathbb{Z}_s$ implies $F_i(\tilde{D}) = s^2 F_i(D)$ for $i = 1, 2, 3$ according to Theorem 4.2 and Proposition 2 of Chen and Tang (2022). This completes the proof. □

To prove Propositions 5.1 and 5.2, the following result from Theorem 1 of Zhou and Tang (2019) is useful.

Lemma A.3. *Suppose that $D = sA + B$ is an $\text{SOA}_s(n, (s^2)^m)$. Then D has orthogonal columns if B is an $\text{OA}(n, m, s, 2)$.*

Proof of Proposition 5.1. Note that the columns of B, which are given by $b_i = \beta_i a_i + e_k \pmod s$ for $i = 1, \ldots, m$, must be distinct columns of a saturated regular $\text{OA}(s^k, (s^k - 1)/(s - 1), s, 2)$ as long as $\beta_i \neq 0$ for $i = 1, \ldots, m$. The result follows immediately from Lemma A.3. □

Proof of Proposition 5.2. Note that B' being an $\text{OA}(s^k, m, s, 2)$ is sufficient for D' being a column orthogonal $\text{SOA}_s(s^k, (s^2)^m)$ according to Lemma A.3. Hence, without loss of generality, it suffices to show that the projection of D onto the first two dimensions, i.e. $(sa_1 + b_1, sa_2 + b_2)$ is of type (iii) if and only if (b'_1, b'_2) is not an $\text{OA}(s^k, 2, s, 2)$. This is straightforward from Theorem 4.2. □

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