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A class of space-filling designs with low-dimensional stratification and column orthogonality

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Abstract: Strong orthogonal arrays are suitable designs for computer experiments because of stratification in low-dimensional projections. However, strong orthogonal arrays may be very expensive for a moderate number of factors. In this article, we develop a method for constructing space-filling designs with more economical run sizes. These designs are not only column-orthogonal but also enjoy a large proportion of low-dimensional stratification properties that strong orthogonal arrays ought to have. Moreover, a class of proposed designs can be 3-orthogonal. In addition, some theoretical results on regular fractional factorial designs are obtained as a by-product.

Résumé: Les tableaux fortement orthogonaux constituent une classe de plans d'expérience bien adaptés aux expérimentations par ordinateur, et ce en raison de la stratification dans les projections en basse dimension. Ils peuvent toutefois être très coûteux même en présence d'un nombre modéré de facteurs. Les auteurs de cet article élaborent une méthode de construction de plans d'expérience comblant l'espace avec des essais de tailles plus économiques. En plus de satisfaire l'orthogonalité entre colonnes, les plans proposés jouissent d'une bonne partie des propriétés de stratification en basse dimension, propriétés que doivent posséder les tableaux fortement orthogonaux. Aussi, certains de ces plans peuvent être 3-orthogonaux. Quelques résultats théoriques concernant des plans factoriels fractionnaires réguliers découlent de l'approche proposée.

1. INTRODUCTION

Computer experiments are widely used in the sciences, engineering, social sciences, and humanities to study complex physical systems. Space-filling designs are common and efficient designs for computer experiments; see Fang, Li & Sudijanto (2006) and Santner, Williams & Notz (2019). In general, a space-filling design is any design whose design points are dispersed over the design area in some uniform manner.

An intuitive approach for constructing space-filling designs is to employ an algorithmic search or a construction method based on a distance or discrepancy criterion; see Johnson, Moore & Ylvisaker (1990) and Fang, Li & Sudijanto (2006) for early work, and Moon, Dean & Santner (2011), Lin & Kang (2016), Wang, Xiao & Xu (2018), and Sun, Wang & Xu (2019) for more recent developments. Inspired by (t, m, s)-nets from quasi-Monte Carlo

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methods (Niederreiter, 1992), He & Tang (2013) introduced and studied strong orthogonal arrays (SOAs). Compared to an ordinary orthogonal array (OA) with the same strength, an SOA has better low-dimensional stratification properties. In order to reduce the cost of the experiment, He & Tang (2014) and He, Cheng & Tang (2018) introduced SOAs of strength 3 and 2+. A computer experiment often involves a large number of factors, especially in the early stages. SOAs, even those with small strength, may still require run sizes that are too large for certain scientific investigations.

Column orthogonality is another important desired property in the design of computer experiments (Bingham, Sitter & Tang, 2009; Wang, Yang & Xu, 2018). There have been a number of studies on orthogonal Latin hypercubes (OLHs), including Steinberg & Lin (2006), Lin, Mukerjee & Tang (2009), Pang, Liu & Lin (2009), Lin et al. (2010), and Sun & Tang (2017), but their run sizes and the number of levels are not flexible enough, and their low-dimensional projections are not as good as those of SOAs. Several research results regarding column-orthogonal strong orthogonal arrays (OSOAs) exist, such as Liu & Liu (2015), Zhou & Tang (2019), and Li, Liu & Yang (2022). However, these OSOAs do not have 3-orthogonality; yet the latter is a good property of designs, being stronger than column orthogonality (Bingham, Sitter & Tang, 2009).

To solve the problems raised in the above two paragraphs, we intend to generate orthogonal designs with economical run sizes that can achieve good low-dimensional space-filling properties. The resulting designs not only enjoy almost the same attractive stratification property in two dimensions as the existing SOAs of strength 2+ but also, as the number of levels is increased from s^2 to s^3, achieve a finer stratification in any one dimension. Moreover, our construction can generate designs with 3-orthogonality that have a relatively high proportion of column triples displaying three-dimensional stratification. In addition, some theoretical properties on orthogonality and regular fractional factorial designs are obtained.

The rest of the article is organized as follows. Section 2 introduces some useful definitions, notation, and preliminaries. Section 3 presents the construction methods and the theoretical properties of the proposed designs. We conclude the article with some discussion in Section 4. All the proofs are provided in the Appendix.

2. NOTATION, DEFINITIONS, AND PRELIMINARIES

An orthogonal array (OA) with n runs, m factors, and strength t is defined as an $n \times m$ array of values, called levels, where column j contains s_j different levels, and for any set of t columns, all combinations of levels occur equally often. We denote such an orthogonal array by $\mathrm{OA}(n, m, s_1 \times \cdots \times s_m, t)$. The simple notation $\mathrm{OA}(n, m, s, t)$ is used for the case $s_1 = \cdots = s_m = s$. In that case, we have $n = \lambda s^t$ for some integer λ, which is called the index of the OA. An $\mathrm{OA}(n, m, s, 1)$ is denoted by $\mathrm{U}(n; s^m)$, and a $\mathrm{U}(n; n^m)$ is called a Latin hypercube design, denoted as $\mathrm{L}(n, m)$.

If there are s^t levels selected from $\{0, \ldots, s^t - 1\}$, then they can be collapsed into s^u levels ($u < t$) by replacing $x \in \{0, \ldots, s^t - 1\}$ with $\lfloor x/s^{t-u_j} \rfloor$, where $\lfloor x \rfloor$ is the largest integer not exceeding x. An $n \times m$ matrix with entries from $\{0, \ldots, s^t - 1\}$ is called a strong orthogonal array of n runs, m factors, s^t levels, and strength t if any g-column subarray with $1 \le g \le t$ can be collapsed into an $\mathrm{OA}(n, g, s^{u_1} \times \cdots \times s^{u_g}, g)$ for any positive integers $u_1, \ldots, u_g$, with $u_1 + \cdots + u_g = t$. We denote such an array by $\mathrm{SOA}(n, m, s^t, t)$. And we say the strong orthogonal array achieves stratification on $s^{u_1} \times \cdots \times s^{u_g}$ grids in some g dimensions if the corresponding g columns of it can be collapsed into an $\mathrm{OA}(n, g, s^{u_1} \times \cdots \times s^{u_g}, g)$. Any $\mathrm{SOA}(n, m, s^t, t)$ can be collapsed into an $\mathrm{OA}(n, m, s, t)$ such that $n = \lambda s^t$, where λ is also called the index of the SOA. Consequently, any $\mathrm{SOA}(n, m, s^3, 3)$ can achieve stratification on $s^2 \times s$ and $s \times s^2$ grids in two dimensions and $s \times s \times s$ grids in three dimensions. We refer readers to He & Tang (2013, 2014) for more details on SOAs.

An $n \times m$ matrix with entries from $\{0, \ldots, s^2 - 1\}$ is called a strong orthogonal array of strength 2+ with n runs and m factors of s^2 levels, denoted by SOA$(n, m, s^2, 2+)$, if any subarray of two columns can be collapsed into an OA$(n, 2, s^2 \times s, 2)$ and an OA$(n, 2, s \times s^2, 2)$. An SOA of strength 2+ enjoys the same attractive two-dimensional space-filling property as that of an SOA of strength 3, while the former has a larger number of factors. An SOA$(n, m, s^2, 2+)$ is said to have strength three minus (3−) if any subarray of three columns can be collapsed into an OA$(n, 3, s, 3)$. We denote this array by SOA$(n, m, s^2, 3-)$. See Zhou & Tang (2019) for more details about SOAs of strength 3−. An $n \times m$ matrix with entries from $\{0, \ldots, s^3 - 1\}$ is called a strong orthogonal array of strength 2∗ with n runs and m factors of s^3 levels, denoted by SOA$(n, m, s^3, 2*)$, if any subarray of two columns can be collapsed into an OA$(n, 2, s^2 \times s, 2)$ and an OA$(n, 2, s \times s^2, 2)$. See Li, Liu & Yang (2022) for more details about SOAs of strength 2∗.

An $r \times c$ matrix with entries from an Abelian group $G = \{\alpha_0, \ldots, \alpha_{s-1}\}$ with $\alpha_0 = 0$ of s elements is called a difference scheme or difference matrix, denoted by D(r, c, s), if it satisfies that for any i and j with $1 \leq i \neq j \leq c$, the vector difference of the ith and jth columns contains every element of G equally often. A difference scheme is said to be normalized if its first column consists of all zeros. For any difference scheme, if we subtract the first column from any column, then we can obtain a normalized difference scheme. Let $A = (a_{ij})$ be an $n_1 \times m_1$ matrix and B be an $n_2 \times m_2$ matrix, where both matrices have entries from an Abelian group G. The Kronecker sum of A and B is an $n_1 n_2 \times m_1 m_2$ matrix given by $A \oplus B = [B^{a_{ij}}]$, where $B^{a_{ij}} = (B + a_{ij})$ is an $n_2 \times m_2$ matrix, with + representing the addition in group G.

Centring a design U(n, s^m) with s equally spaced levels means that the s levels are converted into $x - (s-1)/2$ for $x \in \{0, \ldots, s-1\}$, and then labelled as in the set $\Omega(s) = \{-(s-1)/2, -(s-3)/2, \ldots, (s-3)/2, (s-1)/2\}$. For example, the levels are $-1/2, 1/2$ if $s = 2$ and $-1, 0, 1$ if $s = 3$.

A design U(n, s^m) is called column-orthogonal if the inner product of any two columns of the centred design is zero, denoted by COD(n, s^m). The s levels of a design may be either from an Abelian group G or from $\Omega(s)$. Which is being used should be clear from the context. A COD that is also an SOA is called an orthogonal strong orthogonal array (OSOA). Similarly, a COD that is also a L(n, m) is called an orthogonal Latin hypercube design, denoted as OLH(n, m).

For convenience, a design U(n, s^m) is said to enjoy the two-dimensional and three-dimensional stratification property if it can achieve stratification on $s^2 \times s$ and $s \times s^2$ grids in two dimensions and $s \times s \times s$ grids in three dimensions. We use π and μ to denote the proportion of two-dimensional and three-dimensional stratification, respectively.

3. CONSTRUCTION METHODS

We construct a class of space-filling designs with orthogonality and a high proportion of two-dimensional stratification in this section. A subclass of designs can be 3-orthogonal (3-orthogonality will be discussed in Section 3.2) and have a high proportion of three-dimensional stratification. Some theoretical results related to the properties of the proposed designs are also given in this section.

3.1. General Construction Method

In this subsection, we present the general approach for the construction of a low-dimensional stratification design based on an $A = \text{OA}(n, m, s, 2)$ and a difference scheme $D = \text{D}(r, c, s)$. The key to the construction is to arrange and group the columns of $A \oplus D$ in a proper way. The construction depends on the parity of c. We describe the construction in several steps.

Construction 1. *Let $A = (a_1, \ldots, a_m)$ be an OA$(n, m, s, 2)$, $m \geq 2$, and let $D = (d_1, \ldots, d_c)$ be a normalized difference scheme D(r, c, s) with $c \geq 2$. The levels of both A and D are taken from* *an Abelian group $G = \{\alpha_0, \ldots, \alpha_{s-1}\}$ with $\alpha_0 = 0$. 0_n denotes an n-dimensional column vector with all entries zeros. The following steps present a construction for $Q^* = COD(rn, (s^3)^{4g})$ with $g = \lfloor cm/4 \rfloor$.*

Step 1. *Create*

$$B_i = a_i \oplus D = (a_i \oplus d_1, \ldots, a_i \oplus d_c), \;\; for\ i \in \{1, \ldots, m\}.$$

Divide each B_i into u or $u + 1$ blocks for $i \in \{1, \ldots, m\}$ as

$$B_i = \begin{cases} (B_{i,1}, \ldots, B_{i,u}) & \text{if } c = 2u, \\ (\ell_i, B_{i,1}, \ldots, B_{i,u}) & \text{if } c = 2u + 1, \end{cases}$$

where $\ell_i = a_i \oplus d_1 = a_i \oplus 0_r$, and each block $B_{i,j}$, $j \in \{1, \ldots, u\}$ is composed of two adjacent columns in order from matrix B_i.

Step 2. *(i) If c is even, we have*

$$\begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_m \end{pmatrix} = \begin{pmatrix} B_{1,1} & B_{1,2} & \cdots & B_{1,u} \\ B_{2,1} & B_{2,2} & \cdots & B_{2,u} \\ \vdots & \vdots & \ddots & \vdots \\ B_{m,1} & B_{m,2} & \cdots & B_{m,u} \end{pmatrix},$$

and we order the mu blocks $B_{i,j}$ by column as

$$B_{1,1}, B_{2,1}, \ldots, B_{m,1};\; B_{1,2}, \ldots, B_{m,2};\; \ldots;\; B_{1,u}, \ldots, B_{m,u}.$$

The last block $B_{m,u}$ is deleted if cm is not a multiple of 4; then, we obtain

$$B_{1,1}, B_{2,1}, \ldots, B_{m,1};\; B_{1,2}, \ldots, B_{m,2};\; \ldots;\; B_{1,u}, \ldots, B_{m',u}, \tag{1}$$

where $m' = m$ if cm is a multiple of 4, otherwise $m' = m - 1$.
(ii) If c is odd, we have

$$\begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_m \end{pmatrix} = \begin{pmatrix} \ell_1 & B_{1,1} & B_{1,2} & \cdots & B_{1,u} \\ \ell_2 & B_{2,1} & B_{2,2} & \cdots & B_{2,u} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ell_m & B_{m,1} & B_{m,2} & \cdots & B_{m,u} \end{pmatrix}.$$

Let $L = (\ell_1, \ldots, \ell_m)$. We delete the last $k = cm (\mathrm{mod}\ 4)$ columns of L and rearrange the remaining $m - k$ columns into $(m - k)/2$ pairs as follows:

$$L_1 = (\ell_{i_1}, \ell_{i_2}), \ldots, L_v = (\ell_{i_{2v-1}}, \ell_{i_{2v}}), \ldots, L_{(m-k)/2} = (\ell_{i_{m-k-1}}, \ell_{i_{m-k}}) \tag{2}$$

such that $i_{2v-1}, i_{2v} \neq (m + k)/2 + v$ for $v \in \{1, \ldots, (m - k)/2\}$. Then, order the $(cm - k)/2$ blocks as

$$\begin{aligned} &B_{1,1}, B_{2,1}, \ldots, B_{m,1};\; B_{1,2}, \ldots, B_{m,2};\; \ldots;\; B_{1,u-1}, \ldots, B_{m,u-1}; \\ &\quad B_{1,u}, \ldots, B_{(m+k)/2,u};\; B_{(m+k)/2+1,u},\; L_1,\; \ldots,\; B_{m,u},\; L_{(m-k)/2}. \end{aligned} \tag{3}$$

Step 3. *Map the s levels of (1) and (3) to elements of* $\Omega(s)$, *and denote the resulting design as* $\boldsymbol{B}_i^*, \boldsymbol{B}_{i,j}^*, \boldsymbol{L}_i^*$ *and* $\boldsymbol{\ell}_i^*$. *Take two successive blocks at a time in the order given in (1) or (3), and obtain g sets of four columns, where* $g = \lfloor cm/4 \rfloor$. *Let these sets be* $\boldsymbol{B}^{(1)}, \ldots, \boldsymbol{B}^{(g)}$, *and further let*

$$\boldsymbol{B}^* = \left(\boldsymbol{B}^{(1)}, \ldots, \boldsymbol{B}^{(g)}\right). \tag{4}$$

Step 4. *Define*

$$\boldsymbol{Q}^* = \left(\boldsymbol{Q}^{(1)}, \ldots, \boldsymbol{Q}^{(g)}\right), \tag{5}$$

where $\boldsymbol{Q}^{(j)} = \boldsymbol{B}^{(j)}V$ *for* $j \in \{1, \ldots, g\}$, *and*

$$V = \begin{pmatrix} s^2 & -s & -1 & 0 \\ s & s^2 & 0 & 1 \\ 1 & 0 & s^2 & -s \\ 0 & -1 & s & s^2 \end{pmatrix}.$$

For the design $\boldsymbol{Q}^*$ in (5), we can obtain some theoretical properties, as shown below.

Theorem 1. *If an* OA$(n, m, s, 2)$ *and a difference scheme* D(r, c, s) *exist, then the design* $\boldsymbol{Q}^*$ *in* (5) *is a* COD$(rn, (s^3)^{4g})$ *with* $g = \lfloor cm/4 \rfloor$ *and has the following properties*:

(i) *any two columns achieve stratification on* $s \times s$ *grids*;
(ii) *the proportion* π *of pairs of columns that achieve two-dimensional stratification is at least* π_0 *with*

$$\pi_0 = \begin{cases} \frac{(c-1)(m-1)(cm+m-2k)}{(cm-k)(cm-k-1)} & \text{when } c \text{ is odd;} \\ \frac{(cm-2k)(cm-c)}{(cm-k)(cm-k-1)} & \text{when } c \text{ is even.} \end{cases} \tag{6}$$

By Theorem 1, we know that the design generated by Construction 1 achieves the stratification on $s \times s$ grids in any two dimensions and enjoys column orthogonality. Meanwhile, the proportion of stratification on $s^2 \times s$ and $s \times s^2$ grids is very high in most cases. Table A1 provides some designs generated by Construction 1. It can be seen that $\pi_0 \geq 80\%$ in most cases. Moreover, the bounds π_0 in (6) may not be tight, and the true two-dimensional stratification proportion π of the generated design is possibly higher than π_0 in (6); see Table A1 for details.

Corollary 1 clearly illustrates that we have a large π_0 when m is large, which is the special case of Theorem 1 for the case of c being even and cm being a multiple of 4.

Corollary 1. *If an* OA$(n, m, s, 2)$ *and a difference scheme* D(r, c, s) *exist, where c is even and cm is a multiple of 4, then the design* $\boldsymbol{Q}^*$ *in (5) is a* COD$(rn, (s^3)^{cm})$ *with the proportion of pairs of columns achieving stratification on* $s^2 \times s$ *and* $s \times s^2$ *grids being at least*

$$\pi_0 = \frac{c(m-1)}{cm-1} = 1 - \frac{c-1}{cm-1} \geq 1 - \frac{1}{m}.$$

The following remark is based on Corollary 1.

Remark 1. Any column $q \in Q^*$ can be written as $q = xs^2 \pm ys \pm z$, where $(x, y) \in B^*_{i,j}$, $z \in B^*_{\ell,w}$, and $i \neq \ell$, and this means that x and y must be from the same block, but z needs to be from a different block.

(i) Suppose $q_1 = x_1 s^2 \pm y_1 s \pm z_1$, $q_2 = x_2 s^2 \pm y_2 s \pm z_2$ and $(x_1, y_1) \in B^*_{i_1,j_1}$, $(x_2, y_2) \in B^*_{i_2,j_2}$. Note that q_1 and q_2 can achieve stratification on $s^2 \times s$ and $s \times s^2$ grids if $i_1 \neq i_2$. Thus the design Q^* is a class of strong group-orthogonal arrays (Wang, Yang & Liu, 2022).

(ii) Take $q_w = x_w s^2 \pm y_w s \pm z_w$ from Q^* such that all i_ws are distinct, where $(x_w, y_w) \in B^*_{i_w,j_w}$. By collecting all these q_ws, we can obtain an OSOA$(rn, m, s^3, 2*)$. This method generalizes the result of Li, Liu & Yang (2022), where they derive an OSOA$(sn, 2\lfloor m/2 \rfloor, s^3, 2*)$ based on an OA$(n, m, s, 2)$.

(iii) When c is even and cm is not a multiple of 4, according to (1), we need to delete $k = 2$ columns of $B_{m,u}$. On the basis of (6), the proportion of pairs that achieve stratification on $s^2 \times s$ and $s \times s^2$ grids is at least

$$\pi_0 = \frac{(cm - c)(cm - 4)}{(cm - 2)(cm - 3)} = \left(1 - \frac{c - 2}{cm - 2}\right)\left(1 - \frac{1}{cm - 3}\right)$$
$$\geq 1 - \frac{c - 2}{cm - 2} - \frac{1}{cm - 3}.$$

As Construction 1 is somewhat technical, we present examples to illustrate the main idea. First, we consider the case of an even c.

Example 1.

(i) We now construct a COD$(64, 64^{20})$. Take $A = (a_1, \ldots, a_5)$ as an OA$(16, 5, 4, 2)$ and $D = (d_1, \ldots, d_4)$ as a normalized difference scheme D$(4, 4, 4)$. By Step 1 of Construction 1, we have $B_i = a_i \oplus D = (B_{i,1}, B_{i,2})$, where $B_{i,1} = (a_i \oplus d_1,\ a_i \oplus d_2)$, $B_{i,2} = (a_i \oplus d_3,\ a_i \oplus d_4)$, for $i \in \{1, \ldots, 5\}$. Here, cm is a multiple of 4 and $k = 0$. Then, arrange these columns according to (1), i.e.,

$$B_{1,1}, B_{2,1};\ B_{3,1}, B_{4,1};\ B_{5,1}, B_{1,2};\ B_{2,2}, B_{3,2};\ B_{4,2}, B_{5,2}.$$

Next, map the levels $\{0, 1, 2, 3\}$ of $B_{i,j}$ to $\{-3/2, -1/2, 1/2, 3/2\}$; we obtain $B^*_{i,j}$, $i \in \{1, \ldots, 5\}$, and $j \in \{1, 2\}$. Then, we have

$$Q^* = \left\{Q^{(1)}, Q^{(2)}, Q^{(3)}, Q^{(4)}, Q^{(5)}\right\} = \left\{\left(B^*_{1,1}, B^*_{2,1}\right)V,\ \left(B^*_{3,1}, B^*_{4,1}\right)V,\right.$$
$$\left.\left(B^*_{5,1}, B^*_{1,2}\right)V,\ \left(B^*_{2,2}, B^*_{3,2}\right)V,\ \left(B^*_{4,2}, B^*_{5,2}\right)V\right\}$$

is a COD$(64, 64^{20})$ with $\pi_0 = 84.21\%$. Besides, COD$(64, 64^{20})$ is an OLH$(64, 20)$.

(ii) We construct a COD$(48, 8^{44})$ via Construction 1 based on A = OA$(12, 11, 2, 2)$ and D = D$(4, 4, 2)$. Note that $k = 0$ here, and $\pi_0 = 93.02\%$. It can be checked that the COD$(48, 8^{44})$ listed in Table A1 has a higher two-dimensional stratification proportion of 97.67%.

Example 1 illustrates the case in which c in Construction 1 is even. Although the basic idea of Construction 1 is related to the approach of Sun & Tang (2017), our new method enjoys several advantages. When the run size is s^3, the design resulting from our method is an OLH and includes more columns than an OLH obtained using Theorem 2 of Sun & Tang (2017). The

OLH(64, 20) in Example 1 has four more columns than the OLH(64, 16) obtained by Sun & Tang (2017). In addition, our run size is not necessarily a power of s, but is more flexible, so our method can be used to construct a broader class of orthogonal designs than just OLHs. Most importantly, the method produces designs that are space-filling in low dimensions.

When c is odd, accumulating more columns in the design depends on careful arrangement of the columns in L. As shown in Equation (2), according to Lemma A2 (ii) (in the Appendix), columns paired in L require the condition that $i_{2v-1}, i_{2v} \neq (m+k)/2 + v$ for $v \in \{1, \dots, (m-k)/2\}$, which guarantees that $[B_{(m+k)/2+1,u}, L_1]$ and $[B_{m,u}, L_{(m-k)/2}]$ in Equation (3) are OAs of strength 3.

Next, we consider an example to illustrate the idea.

Example 2.

(i) This example constructs a COD$(27, 27^{12})$. Let $A = (a_1, \dots, a_4)$ be an OA(9, 4, 3, 2), and let $D = (d_1, d_2, d_3)$ be a normalized difference scheme D(3, 3, 3). From Step 1 of Construction 1, we can obtain $B_i = a_i \oplus D = (\ell_i, B_{i,1})$, where $\ell_i = a_i \oplus d_1$, $B_{i,1} = (a_i \oplus d_2,\ a_i \oplus d_3)$, with $i \in \{1, \dots, 4\}$. Here, $m = 4, c = 3, k = 12 (\text{mod } 4) = 0$. Based on (2), we can take $L_1 = (\ell_2, \ell_4), L_2 = (\ell_1, \ell_3)$. Order the six pairs as

$$B_{1,1},\ B_{2,1};\ B_{3,1},\ (\ell_2, \ell_4);\ B_{4,1},\ (\ell_1, \ell_3).$$

After mapping the levels $\{0, 1, 2\}$ to $\Omega(s) = \{-1, 0, 1\}$, we have $B^*_{i,1}$ and $\ell^*_i, i \in \{1, \dots, 4\}$. Then

$$Q^* = \left[Q^{(1)}, Q^{(2)}, Q^{(3)}\right] = \left[(B^*_{1,1},\ B^*_{2,1})V,\ (B^*_{3,1},\ \ell^*_2, \ell^*_4)V,\ (B^*_{4,1},\ \ell^*_1, \ell^*_3)V\right]$$

is a COD$(27, 27^{12})$. When projecting on any two columns, the design can achieve stratification on 3×3 grids, and the proportion of stratification on 9×3 and 3×9 grids is 72.73%. In addition, COD$(27, 27^{12})$ is an OLH(27, 12).

(ii) We now derive a COD$(54, 27^{20})$ from an OA(18, 7, 3, 2) and a normalized D(3, 3, 3). Take OA(18, 7, 3, 2) and D(3, 3, 3) as $A = (a_1, \dots, a_7)$ and $D = (d_1, d_2, d_3)$, respectively. According to Construction 1, we have

$$\begin{pmatrix} \ell_1^\top & \ell_2^\top & \ell_3^\top & \ell_4^\top & \ell_5^\top & \ell_6^\top & \ell_7^\top \\ B_{1,1}^\top & B_{2,1}^\top & B_{3,1}^\top & B_{4,1}^\top & B_{5,1}^\top & B_{6,1}^\top & B_{7,1}^\top \end{pmatrix}^\top,$$

where $\ell_i = a_i \oplus d_1,\ B_{i,1} = (a_i \oplus d_2,\ a_i \oplus d_3),\ i \in \{1, \dots, 7\}$. Here, $m = 7, c = 3, k = 21 (\text{mod } 4) = 1$, and we delete the column ℓ_7 and take $L_1 = (\ell_1, \ell_2), L_2 = (\ell_3, \ell_4), L_3 = (\ell_5, \ell_6)$ based on (2). Order these pairs as

$$B_{1,1},\ B_{2,1};\ B_{3,1},\ B_{4,1};\ B_{5,1},\ (\ell_1, \ell_2);\ B_{6,1},\ (\ell_3, \ell_4);\ B_{7,1},\ (\ell_5, \ell_6).$$

After mapping the levels $\{0, 1, 2\}$ to $\Omega(s) = \{-1, 0, 1\}$, we have $B^*_{i,1}$ and $\ell^*_i, i \in \{1, \dots, 7\}$. Then

$$\begin{aligned} Q^* =& \left\{Q^{(1)}, Q^{(2)}, Q^{(3)}, Q^{(4)}, Q^{(5)}\right\} = \left\{\left(B^*_{1,1},\ B^*_{2,1}\right)V,\ \left(B^*_{3,1},\ B^*_{4,1}\right)V,\right. \\ & \left.(B^*_{5,1},\ \ell^*_1, \ell^*_2)V,\ (B^*_{6,1},\ \ell^*_3, \ell^*_4)V,\ (B^*_{7,1},\ \ell^*_5, \ell^*_6)V\right\} \end{aligned}$$

is a COD$(54, 27^{20})$ with $\pi_0 = 82.11\%$.

For given run sizes, the designs derived in Construction 1 can accommodate more factors than SOAs with strength 2+ (He, Cheng & Tang, 2018) or 3− (Zhou & Tang, 2019). Given an OA$(n, m, s, 2)$, Li, Liu & Yang (2021) presented a construction for COD$\left(sn, (s^2)^{2\lfloor s/2\rfloor m}\right)$. Compared with their designs, the designs derived in Construction 1 can have more levels, more flexible run sizes, more factors, and 3-orthogonality. For example, comparing our COD$(27, 27^{12})$ in Example 2 with COD$(27, 9^8)$, we see that our method gives $s^3 = 27$ levels versus their $s^2 = 9$ and 12 factors rather than 8. Moreover, our method provides a large proportion of stratification in three dimensions as will be discussed in the following subsections. Wang, Yang & Liu (2021) also generated designs from an OA and a difference matrix, but compared with their design COD$\left(sn, (s^3)^{4\lfloor ms'/2\rfloor}\right)$ with $s' = \lfloor s/2\rfloor$, our design enjoys the advantage of accommodating more factors.

3.2. 3-Orthogonal Property

A column orthogonal design $X = (x_{ij})_{n\times m}$ with levels taken from $\Omega(s)$ is said to be 3-orthogonal if

$$\sum_{i=1}^{n} x_{ij_1} x_{ij_2} x_{ij_3} = 0 \ \text{ for } \ j_1 \le j_2 \le j_3.$$

Moreover, 3-orthogonality is used to measure the goodness of a design (Bingham, Sitter & Tang, 2009). A design X with centred levels is said to be mirror-symmetric if $X = -X$ up to row permutations. A column-orthogonal mirror-symmetric design must be 3-orthogonal.

The next result can be derived from Theorem 1 of Sun, Pang & Liu (2011).

Lemma 1. *Let A be a 3-orthogonal matrix and R be a column-orthogonal matrix. Then, AR is a 3-orthogonal matrix.*

For subsequent discussion, we now introduce regular fractional factorial designs. An OA$(s^{m-p}, m, s, 2)$ with levels taken from Galois field GF(s) is said to be regular (Cheng, 2014) if its runs are the solution sets of equations

$$c_i^T x = b_i, \ i \in \{1, \dots, p\}$$

on GF(s), where $c_1, \dots, c_p$ are linearly independent m-dimensional vectors, and $b_1, \dots, b_p \in$ GF(s).

Lemma 2. *Suppose A is an* OA$(s^{m-p}, m, s, 2)$ *with levels taken from* GF$(s) = \{\alpha_0, \dots, \alpha_{s-1}\}$ *with $\alpha_0 = 0$, and*

$$D = \underbrace{D_0 \oplus \cdots \oplus D_0}_{w \text{ times}}, \tag{7}$$

where $D_0 = hh^\top$ and $h = (\alpha_0, \dots, \alpha_{s-1})^\top$.

If A is regular, then $D \oplus A$ is a regular OA$(s^{m_w - p_w}, s^w m, s, 2)$*, with $m_w = s^w m$ and $p_w = m(s^w - 1) + p - w$.*

Theorem 3 of Tang & Xu (2014) states that a regular OA$(n, m, s, 2)$ with s an odd prime can be made mirror-symmetric by permuting the levels of the design. As a consequence, we have following result:

Theorem 2. *If A in Construction 1 is a regular* OA$(n, m, s, 2)$ *with s an odd prime and the levels taken from $\{0, \dots, s-1\}$, and the difference scheme* D *defined as in Equation (7), then Q^* in (5) can be a 3-orthogonal* COD$(s^w n, (s^3)^{4g})$ *with $g = \lfloor s^w m/4\rfloor$.*

TABLE 1: Some CODs with 3-orthogonality.

	Source design			
COD(n, s^m)	Design A	Design D	L(n_1, m_1)	$\pi'_0(\%)$
COD$(125, 125^{56})$	OA$(25, 6, 5, 2)$	D$(5, 5, 5)$	L$(5, 2)$	83.12
COD$(625, 125^{304})$	OA$(125, 31, 5, 2)$	D$(5, 5, 5)$	L$(5, 2)$	93.80
COD$(729, 729^{352})$	OA$(81, 10, 9, 2)$	D$(9, 9, 9)$	L$(9, 4)$	89.51
COD$(1331,1331^{396})$	OA$(121, 12, 11, 2)$	D$(11, 11, 11)$	L$(11, 3)$	91.14
COD$(2197,2197^{540})$	OA$(169, 14, 13, 2)$	D$(13, 13, 13)$	L$(13, 3)$	92.62

Note: Here, π'_0 is the proportion of pairs that achieve stratification on $s^2 \times s$ and $s \times s^2$ grids. Design A comes from the Rao−Hamming construction (Hedayat, Sloane & Stufken, 1999). L$(5, 2)$, L$(9, 4)$ come from Sun, Liu & Lin (2009), and L$(11, 3)$, L$(13, 3)$ come from Wang et al. (2018). By computer search, OA(729,90,9,2) obtained from OA$(81, 10, 9, 2)$ and D$(9, 9, 9)$ can be 3-orthogonal.

According to Theorem 2, we can easily see that the COD$(27, 27^{12})$ in Example 2 can be 3-orthogonal; see Table A2.

Next, we consider constructing a 3-orthogonal design with a greater number of factors than the design in Theorem 2. First, we need the following lemma:

Lemma 3. *Suppose E is an* OA$(n, m, s, 2)$ *and F is an* OLH(s, d). *For $i \in \{1, \dots, d\}$, define the matrix $E^{(i)}$ by replacing the level x of E with F_{xi}. Then*

$$E^* = (E^{(1)}, \dots, E^{(d)})$$

is a COD(n, s^{dm}). *Further, if both E and F are mirror-symmetric, E^* is also mirror-symmetric and 3-orthogonal.*

The following corollary combines Construction 1 and Lemma 3.

Corollary 2. *If a regular* OA$(n, m, s, 2)$ *and an orthogonal mirror-symmetric* L(s, d) *with s an odd prime exist, then for any integer $w \geq 1$, a 3-orthogonal* COD$(s^w n, (s^3)^{4gd})$ *with $g = \lfloor s^w m/4 \rfloor$ can be constructed by combining Theorem 2 and Lemma 3. Additionally, the proportion of pairs that achieve stratification on $s^2 \times s$ and $s \times s^2$ grids is at least π'_0 with*

$$\pi'_0 = \frac{d(c-1)(m-1)(cm+m-2k)}{(cm-k)[d(cm-k)-1]},$$

where $c = s^w$.

Some CODs with 3-orthogonality generated by Theorem 2 and Corollary 2 are shown in Table 1, and the proportions of pairs that achieve stratification on $s^2 \times s$ and $s \times s^2$ grids for these designs are relatively high. In addition, our designs enjoy a larger number of factors compared with those found in the existing SOA-related literature. Next, we explain the above ideas with an example.

Example 3. Let A be a regular OA $(25, 6, 5, 2)$ from the Rao−Hamming construction (Hedayat, Sloane & Stufken, 1999), and $D = hh^\top$ with $h = (0, 1, 2, 3, 4)^\top$, where the operations are modulo 5. Then, $A \oplus D$ is a regular OA $(125, 30, 5, 2)$ (refer to Lemma 2), and we can obtain a mirror-symmetric OA $(125, 30, 5, 2)$ (Theorem 3 of Tang & Xu (2014). By (4) in Construction 1, we can obtain a mirror-symmetric $B^* =$ OA $(125, 28, 5, 2)$. Applying Corollary 2, and noting that an orthogonal mirror-symmetric L $(5, 2)$ can be found in Sun, Liu & Lin (2009), we can obtain a 3-orthogonal COD $(125, 125^{56})$ with $\pi'_0 = 83.12\%$.

3.3. Three-Dimensional Stratification Property

In Theorem 1, we give the two-dimensional stratification property of the proposed designs. Next, we discuss the three-dimensional stratification property of Q^* in (5). We are ready to present the next theorem.

Theorem 3. *In Construction 1, if A is a regular* OA $(n, m, s, 2)$ *and D is defined in (7), the proportion of Q^* in (5) to achieve stratification on $s \times s \times s$ grids is at least $\mu_0 = (4g - s - 1)/(4g - 2)$, where $g = \lfloor s^w m/4 \rfloor$.*

The idea of Corollary 3 is similar to that of Corollary 2.

Corollary 3. *Suppose a regular* OA $(n, m, s, 2)$ *and an* OLH (s, d) *exist; then,* COD $(s^w n, (s^3)^{4gd})$ *can be generated by combining Theorem 3 and Lemma 3, and the proportion of triples that achieve stratification on $s \times s \times s$ grids is at least μ'_0 with*

$$\mu'_0 = \frac{d^2(4g - 1)(4g - s - 1)}{(4gd - 1)(4gd - 2)},$$

where $g = \lfloor s^w m/4 \rfloor$ and w is a positive integer.

Next, we give two examples based on Theorem 3 and Corollary 3.

Example 4. *The proportion of* COD $(27, 27^{12})$ *constructed in Example 2 to achieve stratification on* $3 \times 3 \times 3$ *grids is at least* 80%.

Example 5. *For the* COD $(125, 125^{56})$ *constructed in Example 3, the proportion that achieves stratification on* $5 \times 5 \times 5$ *grids is at least* 80% *according to Corollary 3.*

From Table A1, we can see that the generated designs all have a larger three-dimensional stratification portion than μ_0 or μ'_0.

4. DISCUSSION AND CONCLUSION

A general method was presented in Section 3 that enables the construction of a rich class of space-filling orthogonal designs. The construction requires only an orthogonal array and a difference matrix. The generated orthogonal designs have merits that achieve very attractive stratification in low-dimensional projections.

If we take an orthogonal array A with strength $t \geq 3$, then the low-dimensional stratification of the design generated via Construction 1 can be improved. For example, if we take an orthogonal array with strength 3, then any three columns $q_\ell = x_\ell s^2 \pm y_\ell s \pm z_\ell$ ($\ell \in \{1, 2, 3\}$) of Q^* can achieve stratification on $s^2 \times s \times s$ and $s \times s^2 \times s$ and $s \times s \times s^2$ grids, where $(x_\ell, y_\ell) \in B^*_{i_\ell, j_\ell}$ and i_1, i_2, i_3 are distinct. This three-dimensional stratification property holds for an SOA with strength 4 (Shi & Tang, 2020). If m is even and $c = 2$, the proportion that achieves this three-dimensional stratification property is at least

$$\theta = \frac{2(m-2)}{2m-1} = 1 - \frac{3}{2m-1} \to 1 \text{ as } m \to \infty.$$

In practical applications, one may need to remove one or more columns of Q^* to obtain another orthogonal design with the same run size. We suggest keeping the number of columns of the group corresponding to $a_i \oplus D$ $(1 \le i \le m)$ as close to equal as possible without reducing the number of groups. In this way, one can obtain a design with good low-dimensional projections.

All final designs generated by different A and D of the same dimensions have the same column orthogonality and low-dimensional projections, as stated in Theorems 1 and 3, and the same 3-orthogonality as guaranteed by Theorem 2. Choosing different A and D provides us with an opportunity to find better designs using some secondary design criteria, such as distance or discrepancy criteria. Further evaluating designs is an important direction we will consider in the future. Moreover, the designs generated in this article can be used as original designs to obtain even larger designs. Combining Example 1(i) (generating orthogonal L(64, 20)) and orthogonal L(4, 2), an orthogonal L(64, 40) can be constructed by the method proposed by Lin, Mukerjee & Tang (2009).

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APPENDIX

To prove Theorem 1, we need the following lemmas.

Lemma A1. *Let* $A = (a_1, \ldots, a_m)$ *be an* OA $(n, m, s, 2)$ *and* $D = (d_1, \ldots, d_c)$ *be a difference scheme* D (r, c, s)*, both based on an Abelian group* $G = \{\alpha_0, \ldots, \alpha_{s-1}\}$ *with* $\alpha_0 = 0$*; then, we have the following results*:

(i) $\left[d_1 \oplus (a_1, a_2),\ d_2 \oplus a_1\right]$ *is an* OA *of strength 3*;

(ii) $\left[a_1 \oplus (d_1, d_2),\ a_2 \oplus d_j\right]$ *is an* OA *of strength 3 for any* $d_j \in D$;

(iii) $\left[d_1 \oplus (a_1, a_2),\ d_j \oplus a_3\right]$ *is an* OA *of strength 3 if* $d_1 = 0_r$ *and* $1 < j \leq c$.

Lemma A2. *For* $B_{i,j}$ *and* $L_v = (\ell_{i_{2v-1}}, \ell_{i_{2v}})$ *defined in Construction 1, we have the following*:

(i) $(B_{i_1,j_1}, B_{i_2,j_2})$ *is an* OA *of strength 3 when* $i_1 \neq i_2$;

(ii) $(B_{i,j}, L_v)$ *is an* OA *of strength 3 when* $i \neq i_{2v-1}, i_{2v}$.

Proof. Item (i) can be obtained by item (ii) of Lemma 1, and item (ii) can easily be verified by the cases (ii) and (iii) in Lemma 1. ■

Proof of Theorem 1. The column-orthogonality and (i) follow from the fact that B^* is an OA and $Q^* = B^* R^*$, where $R^* = \mathrm{diag}(V, \ldots, V)$, with V repeating g times. It is easy to see that any column q of Q^* in (5) has the following form: $q = xs^2 \pm ys \pm z$, where $(x, y) \in B^*_{i,j}$ or L^*_v. The number of levels of Q^* is s^3, according to Lemma 2.

Next, we show the two-dimensional stratification on $s^2 \times s$ and $s \times s^2$ grids of Q^*. We first consider the case where c is odd. The $B^*_{i,j}$s and ℓ^*_is can be divided into four groups as (A.1).

$$\left(\begin{array}{c|cccc} C_3 & & C_1 & & \\ \uparrow & & \uparrow & & \\ \ell^*_1 & B^*_{1,1} & B^*_{1,2} & \cdots & B^*_{1,u} \\ \ell^*_2 & B^*_{2,1} & B^*_{2,2} & \cdots & B^*_{2,u} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ell^*_{m-k} & B^*_{m-k,1} & B^*_{m-k,2} & \cdots & B^*_{m-k,u} \\ \hline \ell^*_{m-k+1} & B^*_{m-k+1,1} & B^*_{m-k+1,2} & \cdots & B^*_{m-k+1,u} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ell^*_m & B^*_{m,1} & B^*_{m,2} & \cdots & B^*_{m,u} \\ \downarrow & & \downarrow & & \\ \text{Deleted} & & C_2 & & \end{array}\right). \tag{A.1}$$

Select two columns $q_w = x_w s^2 \pm y_w s \pm z_w$ $(w = 1, 2)$ randomly from Q^*, and let E be the event, i.e.,

$$\begin{aligned} E &= \left\{q_1 \text{ and } q_2 \text{ achieve stratification on } s^2 \times s \text{ and } s \times s^2 \text{ grids}\right\}, \\ F_1 &= \{(x_1, y_1) \in B^*_{i,j} \in C_1 \text{ in (A.1)}\}, \\ F_2 &= \{(x_1, y_1) \in B^*_{i,j} \in C_2 \text{ in (A.1)}\}, \\ F_3 &= \{(x_1, y_1) \in L^*_v \in C_3 \text{ in (A.1)}\}, \end{aligned}$$

then

$$\Pr(F_1) = \frac{(m-k)(c-1)}{cm-k}, \ \Pr(F_2) = \frac{k(c-1)}{cm-k}, \ \Pr(F_3) = \frac{m-k}{cm-k}.$$

Event E occurring is equivalent to both (x_1, y_1, x_2) and (x_1, x_2, y_2) being orthogonal arrays with strength 3.

Given F_1 and $(x_1, y_1) \in B^*_{i_1,j_1} \in C_1$, if

- $(x_2, y_2) \in B^*_{i_2,j_2}$ and $i_1 \neq i_2$ (refer to (i) of Lemma 2), or
- $(x_2, y_2) = (\ell_{i_{2v-1}}, \ell_{i_{2v}}) \in L^*_v$ and $i_1 \neq i_{2v-1}$ (refer to (i) of Lemma 1 and (ii) of Lemma 2),

then E holds. Thus

$$\Pr(E|F_1) \geq \frac{(m-1)(c-1) + (m-k-1)}{cm-k-1}.$$

Given F_2 and $(x_1, y_1) \in B^*_{i_1,j_1} \in C_2$, if

- $(x_2, y_2) \in B^*_{i_2,j_2}$ and $i_1 \neq i_2$ (refer to (i) of Lemma 2), or
- $(x_2, y_2) = (\ell_{i_{2v-1}}, \ell_{i_{2v}}) \in L^*_v$ (refer to (ii) of Lemma 2),

then E holds. Thus

$$\Pr(E|F_2) \geq \frac{(m-1)(c-1)+(m-k)}{cm-k-1}.$$

Given F_3 and $(x_1, y_1) = (\ell_{i_{2v-1}}, \ell_{i_{2v}}) \in L^*_v \in C_3$, if

- $(x_2, y_2) \in B^*_{i_2,j_2}$ and $i_2 \neq i_{2v-1}$ (refer to (i) of Lemma 1 and (ii) of Lemma 2),

then E holds. Thus

$$\Pr(E|F_3) \geq \frac{(m-1)(c-1)}{cm-k-1}.$$

Based on the law of total probability

$$\begin{aligned}\Pr(E) &= \Pr(F_1)\Pr(E|F_1) + \Pr(F_2)\Pr(E|F_2) + \Pr(F_3)\Pr(E|F_3)\\ &\geq \frac{(c-1)(m-1)(cm+m-2k)}{(cm-k)(cm-k-1)}.\end{aligned}$$

When c is even, the $B^*_{i,j}$s can be divided into two groups C_1 and C_2 as (A.1), and $B^*_{m,u}$ is deleted from C_2 if $k = cm (\bmod\ 4) = 2$.

Similar to the case where c is odd, we have

$$\begin{aligned}\Pr(E) &= \Pr(F_1)\Pr(E|F_1) + \Pr(F_2)\Pr(E|F_2)\\ &\geq \frac{(m-1)c}{cm-k}\,\frac{(m-1)c-k}{cm-k-1} + \frac{c-k}{cm-k}\,\frac{(m-1)c}{cm-k-1}\\ &= \frac{(cm-2k)(cm-c)}{(cm-k)(cm-k-1)}.\end{aligned}$$

■

Proof of Lemma 2. We prove only that $D_0 \oplus A$ is regular; then, the conclusion follows by recurrence.

We now construct $p_1 = m(s-1) + p - 1$ linear independent equations with $m_1 = sm$ variables on GF (s) such that the runs of

$$D_0 \oplus A = \left(0_s \oplus A,\ \alpha_1 h \oplus A,\ \ldots,\ \alpha_{s-1} h \oplus A\right)$$

are solution sets of these equations. Since A is regular, suppose the runs of A are solution sets of linear independent equations

$$c_i^T x = b_i,\ i \in \{1, \ldots, p\},\ \ \text{with } \mathrm{Rank}(C_0) = p \ \text{ and }\ C_0 = (c_1, \ldots, c_p)_{m\times p}.$$

This means $AC_0 = b \oplus 0_{s^{m-p}}$, where $b = (b_1, \ldots, b_p)$.

Create an $m_1 \times p_1$ matrix F defined in $\mathrm{GF}(s) = \{\alpha_0, \dots, \alpha_{s-1}\}$ with $\alpha_0 = 0$,

$$F = (f_1, \dots, f_{p_1}) = \begin{pmatrix} C_0 & E_1 & E_2 & \cdots & E_{s-1} \\ & -E_1 & H_2 & \cdots & H_{s-1} \\ & & D_2 & & \\ & & & \ddots & \\ & & & & D_{s-1} \end{pmatrix} \text{ for } s \geq 3,$$

$$\text{and } F = \begin{pmatrix} C_0 & E_1 \\ & -E_1 \end{pmatrix} \text{ for } s = 2,$$

where

$$E_1 = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -1 & 0 & \cdots & 0 \\ 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 \end{pmatrix}_{m\times(m-1)}, \quad E_i = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & -\frac{\alpha_1}{\alpha_i} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -\frac{\alpha_1}{\alpha_i} \end{pmatrix}_{m\times m},$$

$$H_i = \begin{pmatrix} -\frac{\alpha_i}{\alpha_i-\alpha_1} & -1 & \cdots & -1 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}_{m\times m}, \quad D_i = \begin{pmatrix} \frac{\alpha_1}{\alpha_i-\alpha_1} & 0 & \cdots & 0 \\ 0 & \frac{\alpha_1}{\alpha_i} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{\alpha_1}{\alpha_i} \end{pmatrix}_{m\times m},$$

$i \in \{2, \dots, s-1\}$, and the blanks of F are zeros. Clearly, rank $(F) = m(s-1) + p - 1 = p_1$.

It can be verified that

$$(D_0 \oplus A)F = b^* \oplus 0_{s^{m_1-p_1}}, \text{ where } b^* = (b,\ 0_{p_1-p}^\top).$$

Thus, equations

$$f_i^\top y = b_i,\ i \in \{1, \dots, p\};\ f_i^\top y = 0,\ i \in \{p+1, \dots, p_1\},$$

hold for all runs of

$$D_0 \oplus A = \left(0_s \oplus A,\ \alpha_1 h \oplus A,\ \dots,\ \alpha_{s-1} h \oplus A\right).$$

Then, $D_0 \oplus A$ is a regular $\mathrm{OA}(s^{m_1-p_1}, sm, s, 2)$ with $m_1 = sm$ and $p_1 = m(s-1) + p - 1$ based on the definition of regularity. ∎

Proof of Theorem 3. From Construction 1, we can see that Q^* in (5) becomes B^* in (4) after collapsing the factors into s levels. Therefore, we just need to consider the proportion of triples from B^* in (4) are orthogonal arrays of strength 3. Since B^* is a regular orthogonal array (refer to Lemma 2), for any two different columns b_1^* and b_2^*, where $b_1^*, b_2^* \in B^*$, there are at most $s-1$ columns among all remaining columns that can be represented by the linear combination of b_1^* and b_2^*. Thus, the proportion of Q^* in (5) to achieve stratification on $s \times s \times s$ grids is at least μ_0, with

$$\mu_0 = \frac{4g(4g-1)(4g-2-(s-1))}{4g(4g-1)(4g-2)} = \frac{4g-s-1}{4g-2}.$$

∎

TABLE A1: Some CODs with small run sizes which can be generated by Construction 1.

$\mathrm{COD}(n, s^m)$	Source design: Design A	Source design: Design D	$\pi_0(\%)$ (or π'_0)	$\pi(\%)$	$\mu_0(\%)$ (or μ'_0)	$\mu(\%)$
$\mathrm{COD}(16, 8^{12})$	OA(8, 7, 2, 2)	D(2, 2, 2)	90.91	90.91	90.00	92.73
$\mathrm{COD}(32, 8^{28})$	OA(16, 15, 2, 2)	D(2, 2, 2)	96.30	96.30	96.15	96.58
$\mathrm{COD}(32, 8^{28})$	OA(8, 7, 2, 2)	D(4, 4, 2)	88.89	96.30	96.15	99.60
$\mathrm{COD}(48, 8^{44})$	OA(24, 23, 2, 2)	D(2, 2, 2)	97.67	97.67	-	82.48
$\mathrm{COD}(48, 8^{44})$	OA(12, 11, 2, 2)	D(4, 4, 2)	93.02	97.67	-	99.84
$\mathrm{COD}(64, 8^{60})$	OA(32, 31, 2, 2)	D(2, 2, 2)	98.31	98.31	98.28	98.36
$\mathrm{COD}(80, 8^{76})$	OA(40, 39, 2, 2)	D(2, 2, 2)	98.67	98.67	-	79.58
$\mathrm{COD}(96, 8^{92})$	OA(48, 47, 2, 2)	D(2, 2, 2)	98.90	98.90	-	91.96
$\mathrm{COD}(128, 8^{124})$	OA(64, 63, 2, 2)	D(2, 2, 2)	99.19	99.19	99.18	99.20
$\mathrm{COD}(27, 27^{12})$	OA(9, 4, 3, 2)	D(3, 3, 3)	72.73	72.73	80.00	81.82
$\mathrm{COD}(54, 27^{20})$	OA(18, 7, 3, 2)	D(3, 3, 3)	82.11	82.11	-	78.95
$\mathrm{COD}(54, 27^{24})$	OA(9, 4, 3, 2)	D(6, 6, 3)	78.26	78.26	-	73.37
$\mathrm{COD}(81, 27^{36})$	OA(9, 4, 3, 2)	D(9, 9, 3)	76.19	93.97	94.12	94.79
$\mathrm{COD}(81, 27^{36})$	OA(27, 13, 3, 2)	D(3, 3, 3)	87.62	91.90	94.12	94.75
$\mathrm{COD}(162, 27^{72})$	OA(54, 25, 3, 2)	D(3, 3, 3)	88.26	92.80	-	91.62
$\mathrm{COD}(162, 27^{76})$	OA(27, 13, 3, 2)	D(6, 6, 3)	93.47	93.47	-	91.88
$\mathrm{COD}(64, 64^{20})$	OA(16, 5, 4, 2)	D(4, 4, 4)	84.21	84.21	83.33	84.21
$\mathrm{COD}(128, 64^{36})$	OA(32, 9, 4, 2)	D(4, 4, 4)	91.43	91.43	-	80.67
$\mathrm{COD}(128, 64^{40})$	OA(16, 5, 4, 2)	D(8, 8, 4)	82.05	82.05	-	81.62
$\mathrm{COD}(125, 125^{56})$	OA(25, 6, 5, 2)	D(5, 5, 5)	83.12	83.12	80.00	81.50

Here, π is the true proportion of pairs that achieve stratification on $s^2 \times s$ and $s \times s^2$ grids, and μ is the true proportion of triples that achieve stratification on $s \times s \times s$ grids. We use "-" to indicate that the proportion is not given because the design does not meet the conditions of Theorem 3.

TABLE A2: COD$(27, 27^{12})$

$Q^{(1)}$				$Q^{(2)}$				$Q^{(3)}$			
−13	−5	−11	−7	11	6	−10	4	−1	−1	−6	12
−12	−6	1	−1	−12	−5	−2	−10	−13	−5	−11	−7
−11	−7	13	5	1	−1	12	6	11	6	−10	4
−1	1	−12	−6	−13	−7	−5	11	12	7	−4	−8
0	0	0	0	0	0	0	0	0	0	0	0
1	−1	12	6	13	7	5	−11	−12	−7	4	8
11	7	−13	−5	−1	1	−12	−6	−11	−6	10	−4
12	6	−1	1	12	5	2	10	13	5	11	7
13	5	11	7	−11	−6	10	−4	1	1	6	−12
3	8	3	10	−10	3	−8	3	5	−13	−7	11
4	10	6	−11	3	10	−3	−8	2	10	−12	−5
2	9	−9	4	7	−13	11	5	−10	3	−8	3
6	−13	2	8	2	8	−6	13	−9	4	−2	−9
7	−11	5	−13	6	−12	−1	−1	6	−12	−1	−1
5	−12	−10	2	−8	4	7	−12	3	8	3	10
−9	2	4	9	5	−11	−13	−7	4	9	9	−2
−8	4	7	−12	−9	2	4	9	−8	2	13	6
−10	3	−8	3	4	9	9	−2	7	−11	5	−13
10	−3	8	−3	−4	−9	−9	2	−7	11	−5	13
8	−4	−7	12	9	−2	−4	−9	8	−2	−13	−6
9	−2	−4	−9	−5	11	13	7	−4	−9	−9	2
−5	12	10	−2	8	−4	−7	12	−3	−8	−3	−10
−7	11	−5	13	−6	12	1	1	−6	12	1	1
−6	13	−2	−8	−2	−8	6	−13	9	−4	2	9
−2	−9	9	−4	−7	13	−11	−5	10	−3	8	−3
−4	−10	−6	11	−3	−10	3	8	−2	−10	12	5
−3	−8	−3	−10	10	−3	8	−3	−5	13	7	−11

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