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REGULAR ARTICLE

Several new classes of space-filling designs

Wenlong Li[1] · Min-Qian Liu[2] · Jian-Feng Yang[2]

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Abstract

Mappable nearly orthogonal arrays were recently proposed as a new class of space-filling designs for computer experiments. Inspired by mappable nearly orthogonal arrays, we propose several new classes of space-filling designs. The corresponding construction methods are provided. The resulting designs are more space-filling than mappable nearly orthogonal arrays while accommodating a large number of factors. In addition to the space-filling properties, the column orthogonality is also desirable for designs of computer experiments. Among the new constructed designs, one class is column-orthogonal, and the other two classes, providing many new column-orthogonal designs, are nearly column-orthogonal in the sense that each column is column-orthogonal to a large proportion of the other columns. The constructed designs are good choices for computer experiments due to their attractive space-filling properties and column orthogonality. The proposed construction methods are flexible in the choices of an orthogonal array and/or a strong orthogonal array and their usefulness is appealing. Many newly constructed space-filling designs are tabulated. The expansive replacement method and the generalized doubling play key roles in the constructions.

Keywords Computer experiment · Expansive replacement method · Generalized doubling · Orthogonal array · Stratification

1 Introduction

Computer experiments are powerful tools to investigate the complex phenomena and systems in engineering and sciences. Space-filling designs are most commonly used in computer experiments (Santner et al. 2018; Fang et al. 2006). An appealing approach to find space-filling designs is based on an algorithmic search using a distance (John-

✉ Jian-Feng Yang
jfyang@nankai.edu.cn

[1] School of Mathematics and Statistics, Beijing Institute of Technology, Beijing 100081, China

[2] School of Statistics and Data Science, LPMC & KLMDASR, Nankai University, Tianjin 300071, China

son et al. 1990) or discrepancy criterion (Fang et al. 2018). Although this method is flexible in the selections of an algorithmic criterion as well as the numbers of runs and/or factors, it often becomes ineffective for searching large designs. A more fruitful approach is to utilize some systematic methods to construct designs that are space-filling in low-dimensional projections. Such designs went back to Latin hypercubes (McKay et al. 1979), randomized orthogonal arrays (OAs) (Owen 1992) and OA-based Latin hypercubes (Tang 1993).

Recently, He and Tang (2013) introduced the concept of *strong orthogonal arrays* (SOAs) for computer experiments. Compared with an OA of strength t, an SOA of strength t enjoys better space-filling properties in less than t dimensions while retaining the same space-filling properties in t dimensions. To enjoy attractive space-filling properties of SOAs, its strength should be larger than two. He and Tang (2014) examined the characterization of SOAs of strength 3. Given the number of factors, SOAs of strength 3 require a large number of runs. He et al. (2018) proposed a new class of arrays, called SOAs of strength 2+, which are more economical than SOAs of strength 3 while retaining the two-dimensional space-filling property of the latter. Mukerjee et al. (2014) proposed mappable nearly orthogonal arrays (MNOAs) to seek for attractive low-dimensional space-filling properties as well as a large number of factors. For more recent work about SOAs and MNOAs, see Liu and Liu (2015), Zhou and Tang (2019), Shi and Tang (2019, 2020), Li et al. (2021, 2022), Wang et al. (2022) and Liu et al. (2023).

Motivated by the idea of MNOAs, we present in this paper several new classes of space-filling designs (i.e., Type-I, Type-II and Type-III MNOAs) and provide corresponding construction methods. The resulting designs are useful for computer experiments because they enjoy more space-filling properties than MNOAs while accommodating a large number of factors. In addition to the space-filling properties, the proposed designs possess the property of column orthogonality, which is also desirable for designs of computer experiments. Among the three types of MNOAs, the Type-II MNOAs are column-orthogonal, and the other two types, i.e., Type-I and Type-III MNOAs are nearly column-orthogonal in the sense that each column is column-orthogonal to a large proportion of the other columns. Besides, two theoretical results show that Type-I and Type-III MNOAs provide many new column-orthogonal designs. Having the attractive space-filling properties and column orthogonality, the constructed designs are good choices for computer experiments.

The rest of this paper is organized as follows. Section 2 provides some definitions and preliminaries. Section 3 investigates some construction methods for constructing several new classes of space-filling designs, along with the additional property of column orthogonality. Section 4 contains some concluding remarks. All the proofs are deferred to the Appendix.

2 Definitions and preliminaries

Let $\mathrm{D}(n, s^m)$ denote a balanced design with n runs, m factors, and s levels from $\{0, 1, \ldots, s-1\}$ where the s levels appear equally often for each factor. If $n = s$, then a $\mathrm{D}(n, s^m)$ becomes a Latin hypercube, denoted by $\mathrm{LH}(n, m)$. The centered design is a design whose s levels are equally spaced and labeled as the set $\Omega(s) = \{-(s-1)/2, -(s-3)/2, \ldots, (s-3)/2, (s-1)/2\}$. For example, $\Omega(2) = \{-1/2, 1/2\}$ and $\Omega(3) = \{-1, 0, 1\}$. A D(n, s^m) is called column-orthogonal if the inner product of any two columns of the centered design is zero.

An $n \times m$ matrix with entries from $\{0, 1, \ldots, s_j - 1\}$ in the jth column is an OA of n runs, m factors and strength t if, in any $n \times t$ subarray, all possible level combinations occur equally often. We denote such an array by OA$(n, m, s_1 \times \cdots \times s_m, t)$. When $s_1 = \cdots = s_m = s$, the array is symmetric and denoted by OA(n, m, s, t). In particular for an OA(n, m, s, t) with $t = 2$, we often use a simple notation OA(n, s^m) instead. For an OA(n, s^m), we have $n = \lambda s^2$ for some integer $\lambda \geq 1$. We also use OA$(\lambda s^2, s^m)$ in the rest of the paper. We call the orthogonality for an OA *combinatorial orthogonality*. Obviously, combinatorial orthogonality implies column orthogonality, but this is not necessarily true for the inverse. An $n \times m$ matrix with entries from $\{0, 1, \ldots, s^t - 1\}$ is called an SOA of n runs, m factors, s^t levels and strength t, denoted by SOA(n, m, s^t, t), if any subarray of g columns for any g with $1 \leq g \leq t$ can be collapsed into an OA$(n, g, s^{u_1} \times \cdots \times s^{u_g}, g)$ for any positive integers $u_1, \ldots, u_g$ with $u_1 + \cdots + u_g = t$, where collapsing s^t levels into s^{u_j} levels is according to $\lfloor x/s^{t-u_j} \rfloor$ for $x = 0, 1, \ldots, s^t - 1$, and $\lfloor x \rfloor$ is the largest integer not exceeding x. Consequently, any SOA$(n, m, s^3, 3)$ can achieve stratifications on $s^2 \times s$ and $s \times s^2$ grids in two dimensions and on $s \times s \times s$ grids in three dimensions. For more details about SOAs, we refer to He and Tang (2013; 2014).

Example 1 Consider the SOA(8, 3, 8, 3):

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

where ^{T} denotes the transpose of a matrix. This array has the following properties: (i) the array can be collapsed into an OA(8, 3, 2, 3) when collapsing eight levels into two levels according to $0, 1, 2, 3 \rightarrow 0$; $4, 5, 6, 7 \rightarrow 1$; (ii) any array of two columns can be collapsed into an OA$(8, 2, 4 \times 2, 2)$ or an OA$(8, 2, 2 \times 4, 2)$ when the levels of one factor are collapsed into four levels according to $0, 1 \rightarrow 0$; $2, 3 \rightarrow 1$; $4, 5 \rightarrow 2$; $6, 7 \rightarrow 3$ and the levels of the other factor are collapsed into two levels; (iii) any array of one column is an OA(8, 1, 8, 1).

An $n \times m$ matrix with entries from $\{0, 1, \ldots, s^2 - 1\}$ is called an SOA 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$(n, m, s^2, 2+)$ enjoys the same two-dimensional space-filling property as an SOA$(n, m, s^3, 3)$, while the former can accommodate more factors. An $n \times m$ matrix with entries from $\{0, 1, \ldots, s^3 - 1\}$ is called an SOA of strength 2∗, 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$(n, 2, s \times s^2, 2)$. According to the definitions of SOA$(n, m, s^2, 2+)$ and SOA$(n, m, s^3, 2*)$, their main difference lies in the number of levels, i.e., the former has s^2 levels, while the latter has s^3 levels. We denote a column-orthogonal SOA(n, m, s^t, r) by an OSOA(n, m, s^t, r) with $(t, r) = (3, 3)$, $(2, 2+)$

and (3, 2∗) here. From the definitions, all the OSOA(n, m, s^t, r)'s with distinct t and r have $n = \lambda_1 s^3$ for some integer $\lambda_1 \geq 1$.

An $n \times m_1 m_2$ array with entries from $\{0, 1, \ldots, s-1\}$ is an MNOA, denoted by MNOA$(n, {m_2}^{m_1}, s, p)$ where $s = p^t$ with $t \geq 2$, if it can be partitioned into m_1 disjoint groups each of m_2 columns, and satisfies that any two columns from different groups achieve a stratification on an $s \times s$ grid and any two columns from the same group achieve a stratification on a $p \times p$ grid.

Chen and Cheng (2006) studied the method of doubling for constructing two-level fractional factorial designs. Let X be a D$(n, 2^m)$, the double of X is the $2n \times 2m$ design $\begin{pmatrix} X & X \\ X & 1+X \end{pmatrix}$, where $1 + X$ is the matrix obtained from X by adding 1 to each entry of X (modulo 2). Generally, when design X is a D(n, s^m), define the generalized double of X to be

$$GD(X) = \begin{pmatrix} X & X \\ X & 1+X \\ \vdots & \vdots \\ X & s-1+X \end{pmatrix}, \tag{1}$$

where $u + X$ is the matrix by adding u to all the entries of X (modulo s) for $u = 1, \ldots, s-1$. For convenience of constructions, divide $GD(X)$ into two parts, and denote them as

$$GD_{\mathrm{I}}(X) = (X^T, \ldots, X^T)^T \quad \text{and} \quad GD_{\mathrm{II}}(X) = (X^T, 1+X^T, \ldots, s-1+X^T)^T, \tag{2}$$

respectively. The $GD_{\mathrm{I}}(X)$ and $GD_{\mathrm{II}}(X)$ are very useful for constructing space-filling designs in the next section.

3 Construction methods

This section provides some methods for constructing three new classes of space-filling designs (i.e., Type-I, Type-II and Type-III MNOAs). A common characteristic of the constructions is that they are based on the expansive replacement method (Hedayat et al. 1999). This method is used for the construction of OAs, while we here use the method to construct a space-filling design D$(n, p^{m_1 m_2})$ as stated below and denoted by C.

Let A be a D(n, s^{m_1}) and B be a D(s, p^{m_2}). In each column of A, replace the uth level by the $(u+1)$th row of B for $u = 0, 1, \ldots, s-1$. The resulting matrix C must be a D$(n, p^{m_1 m_2})$, and write

$$C = (C_1, \ldots, C_{m_1}), \tag{3}$$

where $C_i = (c_{i1}, \ldots, c_{im_2})$ is the ith group of m_2 columns obtained by replacing the levels of the ith column of A by the rows of B. An illustrative example is given below.

Table 1 Design A, D(16, 4^5)

1	2	3	4	5
0	0	0	0	0
1	0	1	1	1
2	0	2	2	2
3	0	3	3	3
0	1	1	2	3
1	1	0	3	2
2	1	3	0	1
3	1	2	1	0
0	2	2	3	1
1	2	3	2	0
2	2	0	1	3
3	2	1	0	2
0	3	3	1	2
1	3	2	0	3
2	3	1	3	0
3	3	0	2	1

Table 2 Design B, D(4, 4^3)

1	2	3
0	2	3
1	1	0
2	3	1
3	0	2

Example 2 Let A be a $D(16, 4^5)$ and B be a $D(4, 4^3)$, as shown in Tables 1 and 2. Based on the expansive replacement method, we can obtain a design C by replacing the uth level of A by the $(u+1)$th row of B for $u = 0, 1, 2, 3$. Then $C = (C_1, \ldots, C_5)$ is a $D(16, 4^{15})$, as given in Table 3. Obviously, design C is an MNOA$(16, 3^5, 4, 2)$.

3.1 Type-I MNOAs

This subsection considers the construction of (column-orthogonal) Type-I MNOAs. We first give the following definition. Throughout this paper, we use the notation λ and sometimes the notation λ_1, where $\lambda \geq 1$ and $\lambda_1 \geq 1$ are two integers.

Definition 1 An $n \times m_1 m_2$ array with entries from $\{0, 1, \ldots, s-1\}$ is called a Type-I MNOA, denoted by $\text{MNOA}_{\text{I}}(n, {m_2}^{m_1}, s, p)$ with $s = \lambda_1 p^3$, where $\lambda_1 \geq 1$ is an integer, if it can be partitioned into m_1 disjoint groups each of m_2 columns, and satisfies the following properties:

(a) any two columns from different groups are column-orthogonal;

Table 3 Design C, D(16, 4^{15})

C_1			C_2			C_3			C_4			C_5		
0	2	3	0	2	3	0	2	3	0	2	3	0	2	3
1	1	0	0	2	3	1	1	0	1	1	0	1	1	0
2	3	1	0	2	3	2	3	1	2	3	1	2	3	1
3	0	2	0	2	3	3	0	2	3	0	2	3	0	2
0	2	3	1	1	0	1	1	0	2	3	1	3	0	2
1	1	0	1	1	0	0	2	3	3	0	2	2	3	1
2	3	1	1	1	0	3	0	2	0	2	3	1	1	0
3	0	2	1	1	0	2	3	1	1	1	0	0	2	3
0	2	3	2	3	1	2	3	1	3	0	2	1	1	0
1	1	0	2	3	1	3	0	2	2	3	1	0	2	3
2	3	1	2	3	1	0	2	3	1	1	0	3	0	2
3	0	2	2	3	1	1	1	0	0	2	3	2	3	1
0	2	3	3	0	2	3	0	2	1	1	0	2	3	1
1	1	0	3	0	2	2	3	1	0	2	3	3	0	2
2	3	1	3	0	2	1	1	0	3	0	2	0	2	3
3	0	2	3	0	2	0	2	3	2	3	1	1	1	0

(b) any two columns from different groups achieve a stratification on an $s \times s$ grid;
(c) any two columns from the same group achieve stratifications on $p^2 \times p$ and $p \times p^2$ grids.

From Definition 1(b), in an $\text{MNOA}_{\text{I}}(n, {m_2}^{m_1}, s, p)$, any two columns from different groups form an OA with s levels and then have combinatorial orthogonality; so each column is also column-orthogonal to a large proportion of the other columns. This implies that the measure of the degree of such stratifications and orthogonality among columns can be calculated as

$$\pi = (m_1 - 1)m_2/(m_1 m_2 - 1), \tag{4}$$

which is very high and close to 1 as m_1 gets large. In the next two subsections, one can also use π in (4) to evaluate the column orthogonality and/or stratifications between groups for Type-II and Type-III MNOAs.

We now present the construction of an $\text{MNOA}_{\text{I}}(\lambda s^2, {m_2}^{m_1}, s, p)$, where $\lambda \geq 1$ is an integer.

Construction 1

Step 1. Take A to be an $\text{OA}(\lambda s^2, s^{m_1})$, where $\lambda \geq 1$ is an integer.
Step 2. Based on an $\text{SOA}(s, m_2, p^2, 2+)$ where $s = \lambda_1 p^3$, where $\lambda_1 \geq 1$ is an integer, take B to be an $\text{LH}(s, m_2)$ obtained by, for each column, replacing the $\lambda_1 p$ entries for level j by any permutation of $j\lambda_1 p, j\lambda_1 p + 1, \ldots, (j+1)\lambda_1 p - 1$ for $j = 0, \ldots, p^2 - 1$.
Step 3. Obtain a $\text{D}(\lambda s^2, s^{m_1 m_2})$, say D, using the A and B in Steps 1 and 2 via the expansive replacement method.

Construction 1 is a simple variant of the construction method given by Mukerjee et al. (2014), i.e., the array B becomes an SOA-based Latin hypercube. This change, though simple, leads to a better within-group stratification property, at a price of a smaller factor-to-run ratio. We have the following result.

Theorem 1 *Given an* OA$(\lambda s^2, s^{m_1})$ *and an* SOA$(s, m_2, p^2, 2+)$ *with* $s = \lambda_1 p^3$, *where* $\lambda \geq 1$ *and* $\lambda_1 \geq 1$ *are two integers, the design D in Step 3 of Construction 1 is an* MNOA$_{\text{I}}(\lambda s^2, {m_2}^{m_1}, s, p)$.

Theorem 1 shows that we can obtain a Type-I MNOA when the number of levels for an OA is equal to the run size for an SOA of strength 2+. An illustrative example is presented as follows.

Example 3 Given an OA$(256, 16^{17})$ and an SOA$(16, 10, 4, 2+)$, Construction 1 allows for the construction of an MNOA$_{\text{I}}(256, 10^{17}, 16, 2)$. All 170 columns are partitioned into 17 disjoint groups each of 10 columns such that any two columns from distinct groups achieve a stratification on a 16×16 grid and any two columns from the same group achieve stratifications on 4×2 and 2×4 grids. With $m_1 = 17$ and $m_2 = 10$ in (4), we have the degree of stratifications on 16×16 grids of $\pi = 0.947$. This implies that the property of stratifications in two dimensions is almost the same as that of the OA$(256, 16^{17})$. Compared with this OA of 17 columns, the newly constructed MNOA$_{\text{I}}(256, 10^{17}, 16, 2)$ has 153 more columns. Compared with MNOAs, the MNOA$_{\text{I}}(256, 10^{17}, 16, 2)$ is a compromise between the MNOA$(256, 15^{17}, 16, 2)$ and MNOA$(256, 5^{17}, 16, 4)$ in Mukerjee et al. (2014).

Table 4 provides some new Type-I MNOAs using Theorem 1 based on the existing OAs from Hedayat et al. (1999) and SOAs of strength 2+ from He et al. (2018). Type-I MNOAs have the attractive two-dimensional space-filling property while accommodating a substantially large number of factors. For instance, taking an OA$(512, 16^{33})$ and an SOA$(16, 10, 4, 2+)$ in Theorem 1 gives an MNOA$_{\text{I}}(512, 10^{33}, 16, 2)$ with $\pi = 0.973$, which has 330 factors. If we take an OA$(1024, 32^{33})$ and an SOA$(32, 22, 4, 2+)$, we obtain an MNOA$_{\text{I}}(1024, 22^{33}, 32, 2)$ with $\pi = 0.971$, which can accommodate up to 726 factors. More Type-I MNOAs are listed in Table 4.

We now construct a column-orthogonal Type-I MNOA when the OSOA of strength $2*$ from Li et al. (2022) is used. More specifically, by using an OSOA$(s, m_2, p^3, 2*)$ with $s = p^3$ as B and still using an OA$(\lambda s^2, s^{m_1})$ as A, we have the next result based on Construction 1.

Theorem 2 *Let A be an* OA$(\lambda s^2, s^{m_1})$ *and B be an* OSOA$(s, m_2, p^3, 2*)$ *with* $s = p^3$. *Then a column-orthogonal* MNOA$_{\text{I}}(\lambda s^2, {m_2}^{m_1}, s, p)$ *can be constructed from the A and B via Construction 1.*

Theorem 2 allows Type-I MNOAs with the additional column orthogonality to be constructed. Similar to Tables 4 and 5 lists some new column-orthogonal Type-I MNOAs by Theorem 2 based on suitable choices of OAs for practical use.

Example 4 If we take A to be an OA$(729, 27^{28})$ and B to be an OSOA$(27, 4, 27, 2*)$ in Theorem 2, we can obtain a column-orthogonal MNOA$_{\text{I}}(729, 4^{28}, 27, 3)$ with $\pi =$

Table 4 Some Type-I MNOAs

p	$\mathrm{OA}(\lambda s^2, s^{m_1})$	$\mathrm{SOA}(s, m_2, p^2, 2+)$	Type-I MNOA	π
2	$\mathrm{OA}(64, 8^9)$	$\mathrm{SOA}(8, 3, 4, 2+)$	$\mathrm{MNOA_I}(64, 3^9, 8, 2)$	0.923
2	$\mathrm{OA}(128, 8^{17})$	$\mathrm{SOA}(8, 3, 4, 2+)$	$\mathrm{MNOA_I}(128, 3^{17}, 8, 2)$	0.960
2	$\mathrm{OA}(576, 8^{22})$	$\mathrm{SOA}(8, 3, 4, 2+)$	$\mathrm{MNOA_I}(576, 3^{22}, 8, 2)$	0.969
2	$\mathrm{OA}(256, 16^{17})$	$\mathrm{SOA}(16, 10, 4, 2+)$	$\mathrm{MNOA_I}(256, 10^{17}, 16, 2)$	0.947
2	$\mathrm{OA}(512, 16^{33})$	$\mathrm{SOA}(16, 10, 4, 2+)$	$\mathrm{MNOA_I}(512, 10^{33}, 16, 2)$	0.973
2	$\mathrm{OA}(1024, 32^{33})$	$\mathrm{SOA}(32, 22, 4, 2+)$	$\mathrm{MNOA_I}(1024, 22^{33}, 32, 2)$	0.971
2	$\mathrm{OA}(2048, 32^{65})$	$\mathrm{SOA}(32, 22, 4, 2+)$	$\mathrm{MNOA_I}(2048, 22^{65}, 32, 2)$	0.985
3	$\mathrm{OA}(729, 27^{28})$	$\mathrm{SOA}(27, 6, 9, 2+)$	$\mathrm{MNOA_I}(729, 6^{28}, 27, 3)$	0.970
3	$\mathrm{OA}(1458, 27^{55})$	$\mathrm{SOA}(27, 6, 9, 2+)$	$\mathrm{MNOA_I}(1458, 6^{55}, 27, 3)$	0.985
4	$\mathrm{OA}(4096, 64^{65})$	$\mathrm{SOA}(64, 8, 16, 2+)$	$\mathrm{MNOA_I}(4096, 8^{65}, 64, 4)$	0.987
4	$\mathrm{OA}(8192, 64^{129})$	$\mathrm{SOA}(64, 8, 16, 2+)$	$\mathrm{MNOA_I}(8192, 8^{129}, 64, 4)$	0.993
5	$\mathrm{OA}(15625, 125^{126})$	$\mathrm{SOA}(125, 10, 25, 2+)$	$\mathrm{MNOA_I}(15625, 10^{126}, 125, 5)$	0.993

Table 5 Some column-orthogonal Type-I MNOAs

p	$\mathrm{OA}(\lambda s^2, s^{m_1})$	$\mathrm{OSOA}(s, m_2, p^3, 2*)$	Type-I MNOA	π
3	$\mathrm{OA}(729, 27^{28})$	$\mathrm{OSOA}(27, 4, 27, 2*)$	$\mathrm{MNOA_I}(729, 4^{28}, 27, 3)$	0.973
3	$\mathrm{OA}(1458, 27^{55})$	$\mathrm{OSOA}(27, 4, 27, 2*)$	$\mathrm{MNOA_I}(1458, 4^{55}, 27, 3)$	0.986
4	$\mathrm{OA}(4096, 64^{65})$	$\mathrm{OSOA}(64, 4, 64, 2*)$	$\mathrm{MNOA_I}(4096, 4^{65}, 64, 4)$	0.988
4	$\mathrm{OA}(8192, 64^{129})$	$\mathrm{OSOA}(64, 4, 64, 2*)$	$\mathrm{MNOA_I}(8192, 4^{129}, 64, 4)$	0.994
5	$\mathrm{OA}(15625, 125^{126})$	$\mathrm{OSOA}(125, 6, 125, 2*)$	$\mathrm{MNOA_I}(15625, 6^{126}, 125, 5)$	0.993

0.973. Thus, the new constructed column-orthogonal $\mathrm{MNOA_I}$ $(729, 4^{28}, 27, 3)$ can accommodate 112 columns while having the attractive two-dimensional space-filling properties.

From Theorems 1 and 2, we know that $s = \lambda_1 p^3$ for some integer λ_1, which implies that the minimum run size (λs^2) of a Type-I MNOA is λp^6 via taking $\lambda_1 = 1$. In the next subsection, we will discuss the construction of a new class of MNOA with run size λp^5 less than λp^6.

3.2 Type-II MNOAs

This subsection is devoted to the construction of Type-II MNOAs. Such designs can be obtained via a sequence of steps including the expansive replacement method, generalized doubling, column rearrangement and rotation approach (Sun and Tang 2017b). The resulting designs possess good stratification properties and the column orthogonality. Moreover, these designs are supplementary to Type-I MNOAs in terms of run sizes.

Definition 2 An $n \times m_1 m_2$ array with entries from $\{0, 1, \ldots, p^3-1\}$ is called a Type-II MNOA, denoted by $\mathrm{MNOA_{II}}(n, {m_2}^{m_1}, p^3, p)$, if it can be partitioned into m_1 disjoint groups each of m_2 columns, and satisfies the following properties:

(a) the whole array is column-orthogonal;
(b) any two columns from different groups achieve a stratification on a $p^2 \times p^2$ grid;
(c) any two columns from the same group achieve stratifications on $p^2 \times p$ and $p \times p^2$ grids.

Compared with Definition 1, (i) Definition 2(a) is new; (ii) Definition 2(b) shows that any two columns from different groups achieve a stratification on a $p^2 \times p^2$ grid instead of a $(\lambda_1 p^3) \times (\lambda_1 p^3)$ grid; (iii) Definition 2(c) is the same. A measure defined similarly to π in (4) can be used to evaluate the degree of the stratification property of Definition 2(b). By Definition 2, Type-II MNOAs enjoy the attractive two-dimensional space-filling property and column orthogonality.

We now examine how to construct Type-II MNOAs via a series of steps given below.

Construction 2

Step 1 By applying the expansive replacement method with A being an $\mathrm{OA}(\lambda s^2, s^{m_1})$ and B being an $\mathrm{OA}(s, p^{m_2})$ with $s = \lambda_1 p^2$, where $\lambda \geq 1$ and $\lambda_1 \geq 1$ are two integers, we obtain a design C which is an $\mathrm{OA}(\lambda s^2, p^{m_1 m_2})$.

Step 2 The generalized double of C in (1) is an array of size $\lambda p s^2 \times m_1 m_2$. Let $E = GD_{\mathrm{I}}(C)$ and $F = GD_{\mathrm{II}}(C)$, where s in (2) corresponds to p in F. According to the grouping of the columns of C in (3), write

$$E = (E_1, \ldots, E_{m_1}) \quad \text{and} \quad F = (F_1, \ldots, F_{m_1}),$$

where $E_i = (e_{i1}, e_{i2}, \ldots, e_{im_2})$ and $F_i = (f_{i1}, f_{i2}, \ldots, f_{im_2})$ for $i = 1, \ldots, m_1$.

Step 3 Let $g = (0^T_{\lambda s^2}, 1^T_{\lambda s^2}, \ldots, (p-1)^T_{\lambda s^2})^T$, where v_t is the $t \times 1$ vector of all entries v's ($v = 0, 1, \ldots, p-1$). Let $G_i = (e_{i1}, f_{i2}, \ldots, e_{i(m_2-1)}, f_{im_2}, e_{im_2}, f_{i1})$, and arrange the $2m_1m_2 + 2$ columns among $(E, F, g, 1_{\lambda p s^2})$ as

$$G_1; \ldots; G_{m_1}; g, 1_{\lambda p s^2},$$

where G_i is actually obtained by shifting the elements of $(f_{i1}, e_{i1}, f_{i2}, e_{i2}, \ldots, f_{im_2}, e_{im_2})$. From the list above, we take four columns at a time to obtain $q = \lfloor (2m_1m_2 + 2)/4 \rfloor$ sets of four columns. Because of this, there are no leftover columns if m_1m_2 is odd, and the two columns g and $1_{\lambda p s^2}$ are unselected otherwise, i.e., the selected columns for the construction are the list $G_1; \ldots; G_{m_1}; g, 1_{\lambda p s^2}$ for an odd m_1m_2 and the list $G_1; \ldots; G_{m_1}$ for an even m_1m_2. This is the only difference. Those selected columns will be used for the further construction with no difference. For simplicity, we refer the reader to consider the case of even m_1m_2. Let such q sets of four columns be $G^{(1)}, G^{(2)}, \ldots, G^{(q)}$. For each j, let $H_j = G^{(j)} - (p-1)/2$ be the centered design of $G^{(j)}$.

Step 4 Define

$$D^* = (H_1U, \ldots, H_qU), \quad U = \begin{pmatrix} p^2 & p & 1 & 0 \\ -1 & 0 & p^2 & p \end{pmatrix}^T. \tag{5}$$

We see that any column d^* of D^* has the form: $d^* = ep^2 + e'p \pm e''$ with e being a column of $E^* = E - (p-1)/2$, where we call e the leading column of d^*. By noting that the grouping of $E^* = (E_1^*, \ldots, E_{m_1}^*)$ is the same as that of $E = (E_1, \ldots, E_{m_1})$, we now arrange the first m_1m_2 columns in D^* according to the order of their leading columns in the groups $E_1^*, \ldots, E_{m_1}^*$, and denote these new groups as $D_1^*, \ldots, D_{m_1}^*$.

Step 5 For each i, let $D_i = D_i^* + (p^3-1)/2$, which transforms the levels of D^* from $\Omega(s^3)$ into $\{0, 1, \ldots, s^3-1\}$. Define

$$D = (D_1, \ldots, D_{m_1}), \tag{6}$$

where $D_i = (d_{i1}, \ldots, d_{im_2})$ corresponds to D_i^* and represents the ith group of m_2 columns for $i = 1, \ldots, m_1$.

For an odd m_1m_2 in Construction 2, the last column of H_q is actually unimportant at all. In other words, the all-ones column in the list $G_1; \ldots; G_{m_1}; g, 1_{\lambda ps^2}$ can be replaced by anything since it is unused in the construction of D. For design D in (6), we have the following result.

Theorem 3 *Given an* OA($\lambda s^2, s^{m_1}$) *and an* OA(s, p^{m_2}) *with* $s = \lambda_1 p^2$, *where* $\lambda \geq 1$ *and* $\lambda_1 \geq 1$ *are two integers, the design* D *in* (6) *is an* $\mathrm{MNOA_{II}}(\lambda ps^2, {m_2}^{m_1}, p^3, p)$.

The Type-II MNOAs given in Theorem 3 are similar in spirit to the designs presented by Sun and Tang (2017a), i.e., they are a class of column-orthogonal designs that have the MNOA structure. Theorem 3 provides a rich class of column-orthogonal designs with attractive space-filling properties. Taking $\lambda_1 = 1$ in Theorem 3, we see that the run size of an $\mathrm{MNOA_{II}}(\lambda ps^2, {m_2}^{m_1}, p^3, p)$ is a multiple of p^5 while the run size of a Type-I MNOA is a multiple of p^6. Taking $p = 2$ as an example, a Type-II MNOA can have the run size of 32, while the minimum run size of a Type-I MNOA is 64. So Type-II MNOAs are supplementary to Type-I MNOAs in terms of run sizes. Table 6 shows some new Type-II MNOAs obtained by Theorem 3.

Compared with an OSOA($n, m, p^2, 2+$) obtained from Zhou and Tang (2019), a Type-II MNOA not only retains the stratifications on $p^2 \times p$ and $p \times p^2$ grids and column orthogonality but also enjoys the additional properties as follows: (i) the Type-II MNOA achieves finer stratifications in any one dimension than the OSOA, i.e., the former has p^3 levels while the latter only has p^2 levels; (ii) the Type-II MNOA enjoys better two-dimensional space-filling property because it also achieves stratifications on $p^2 \times p^2$ grids in two dimensions with a high ratio.

Example 5 Applying an OA($16, 4^5$) and an OA($4, 2^3$) as A and B respectively in Construction 2 leads to an $\mathrm{MNOA_{II}}(32, 3^5, 8, 2)$, as shown in Table 7. The detailed steps are given below.

Table 6 Some Type-II MNOAs

p	$\mathrm{OA}(\lambda s^2, s^{m_1})$	$\mathrm{OA}(s, p^{m_2})$	Type-II MNOA	π
2	$\mathrm{OA}(16, 4^5)$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{II}}(32, 3^5, 8, 2)$	0.857
3	$\mathrm{OA}(81, 9^{10})$	$\mathrm{OA}(9, 3^4)$	$\mathrm{MNOA_{II}}(243, 4^{10}, 27, 3)$	0.923
3	$\mathrm{OA}(162, 9^{19})$	$\mathrm{OA}(9, 3^4)$	$\mathrm{MNOA_{II}}(486, 4^{19}, 27, 3)$	0.960
4	$\mathrm{OA}(256, 16^{17})$	$\mathrm{OA}(16, 4^5)$	$\mathrm{MNOA_{II}}(1024, 5^{17}, 64, 4)$	0.952
4	$\mathrm{OA}(512, 16^{33})$	$\mathrm{OA}(16, 4^5)$	$\mathrm{MNOA_{II}}(2048, 5^{33}, 64, 4)$	0.976
5	$\mathrm{OA}(625, 25^{26})$	$\mathrm{OA}(25, 5^6)$	$\mathrm{MNOA_{II}}(3125, 6^{26}, 125, 5)$	0.968

Step 1 By applying the expansive replacement method with A and B above, we obtain a design $C = (C_1, \ldots, C_5)$ which is an $\mathrm{OA}(16, 2^{15})$.

Step 2 Let $E = (C^T, C^T)^T$ and $F = (C^T, 1 + C^T)^T$ (modulo 2), which are two arrays of size 32×15. According to the grouping of the columns of C above, write

$$E = (E_1, \ldots, E_5) \quad \text{and} \quad F = (F_1, \ldots, F_5),$$

where $E_i = (e_{i1}, e_{i2}, e_{i3})$ and $F_i = (f_{i1}, f_{i2}, f_{i3})$ for $i = 1, \ldots, 5$.

Step 3 Let $G_i = (e_{i1}, f_{i2}, e_{i2}, f_{i3}, e_{i3}, f_{i1})$, and arrange the 32 columns among $(E, F, g, 1_{32})$ as

$$G_1; \ldots; G_5; g, 1_{32},$$

where G_i is actually obtained by shifting the elements of $(f_{i1}, e_{i1}, f_{i2}, e_{i2}, f_{i3}, e_{i3})$, $g = (0, \ldots, 0,\ 1, \ldots, 1)^T$ with each of 0 and 1 repeating 16 times, and 1_{32} is a column vector of all ones. From the list above, we take four columns at a time to obtain eight sets of four columns. Let such eight sets be $G^{(1)}, G^{(2)}, \ldots, G^{(8)}$, and further let $H_j = G^{(j)} - 1/2$ for each j.

Step 4 Define

$$D^* = (H_1 U, \ldots, H_8 U), \quad U = \begin{pmatrix} 4 & 2 & 1 & 0 \\ -1 & 0 & 4 & 2 \end{pmatrix}^T.$$

We now arrange the first 15 columns in D^* according to the order of their leading columns in the groups $E_1^*, \ldots, E_5^*$ with $E_i^* = E_i - 1/2$, and denote these new groups as $D_1^*, \ldots, D_5^*$.

Step 5 For each i, let $D_i = D_i^* + 7/2$, which transforms the levels of D^* from $\Omega(8)$ into $\{0, 1, \ldots, 7\}$. Then design $D = (D_1, \ldots, D_5)$ becomes an $\mathrm{MNOA_{II}}(32, 3^5, 8, 2)$, where $D_i = (d_{i1}, d_{i2}, d_{i3})$ for $i = 1, \ldots, 5$.

The stratification properties of the $\mathrm{MNOA_{II}}(32, 3^5, 8, 2)$ can be seen intuitively in Fig. 1, where d_j stands for the jth column of the design. The whole design is column-orthogonal. All 15 columns are partitioned into 5 disjoint groups (denoted

Table 7 The $\text{MNOA}_{\text{II}}(32, 3^5, 8, 2)$ in Example 5

D_1			D_2			D_3			D_4			D_5		
0	1	0	1	0	1	0	1	0	1	0	1	0	1	1
0	1	0	3	7	4	3	7	4	2	7	4	3	7	5
0	1	1	5	3	7	4	2	7	4	3	7	4	2	7
0	1	1	7	4	2	7	4	3	7	4	2	7	4	3
3	7	4	0	0	1	3	7	5	4	3	7	7	4	3
3	7	4	2	7	4	0	1	1	7	4	2	4	2	7
3	7	5	4	3	7	7	4	2	1	0	1	3	7	5
3	7	5	6	4	2	4	2	6	2	7	4	0	1	1
4	2	6	0	0	1	4	2	7	6	4	2	3	7	5
4	2	6	2	7	4	7	4	3	5	3	7	0	1	1
4	2	7	4	3	7	0	1	0	3	7	4	7	4	3
4	2	7	6	4	2	3	7	4	0	0	1	4	2	7
7	4	2	1	0	1	7	4	2	3	7	4	4	2	7
7	4	2	3	7	4	4	2	6	0	0	1	7	4	3
7	4	3	5	3	7	3	7	5	6	4	2	0	1	1
7	4	3	7	4	2	0	1	1	5	3	7	3	7	5
2	3	2	3	2	3	2	3	2	3	2	3	2	3	2
2	3	2	1	5	6	1	5	6	0	5	6	1	5	6
2	3	3	7	1	5	6	0	5	6	1	5	6	0	4
2	3	3	5	6	0	5	6	1	5	6	0	5	6	0
1	5	6	2	2	3	1	5	7	6	1	5	5	6	0
1	5	6	0	5	6	2	3	3	5	6	0	6	0	4
1	5	7	6	1	5	5	6	0	3	2	3	1	5	6
1	5	7	4	6	0	6	0	4	0	5	6	2	3	2
6	0	4	2	2	3	6	0	5	4	6	0	1	5	6
6	0	4	0	5	6	5	6	1	7	1	5	2	3	2
6	0	5	6	1	5	2	3	2	1	5	6	5	6	0
6	0	5	4	6	0	1	5	6	2	2	3	6	0	4
5	6	0	3	2	3	5	6	0	1	5	6	6	0	4
5	6	0	1	5	6	6	0	4	2	2	3	5	6	0
5	6	1	7	1	5	1	5	7	4	6	0	2	3	2
5	6	1	5	6	0	2	3	3	7	1	5	1	5	6

by $D_1, \ldots, D_5$) each of 3 columns such that any two columns (e.g., (d_1, d_4)) from distinct groups achieve a stratification on a 4×4 grid in 90 out of 105 two dimensions and any two columns (e.g., (d_1, d_2)) from the same group achieve stratifications on 4×2 and 2×4 grids in the remaining 15 two dimensions, where d_1 and d_2 belong to group D_1 and d_4 and d_5 belong to group D_2. We now compare Type-II MNOAs and designs in Sun and Tang (2017a). Take the $\text{MNOA}_{\text{II}}(32, 3^5, 8, 2)$ and the $\text{OD}(32, 16^{16})$ in Sun and Tang (2017a) as an example. The former has fewer factors (only by one), but enjoys a better space-filling property, although these two designs do not have the

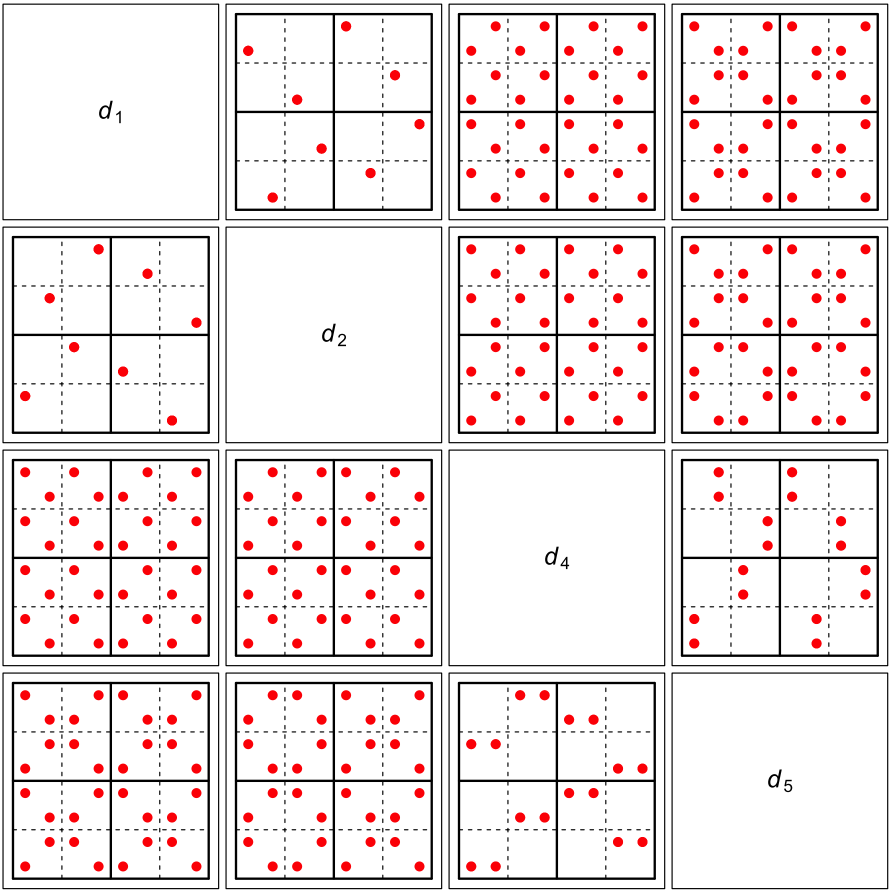

Fig. 1 Bivariate projections of the columns (d_1, d_2, d_4, d_5) of the $\text{MNOA}_{\text{II}}(32, 3^5, 8, 2)$ in Example 5

same number of levels. In general, Type-II MNOAs are of p^3 levels, and the designs in Sun and Tang (2017a) are of p^4 levels.

The SOA(32, 9, 8, 3) in Example 1 from Shi and Tang (2020) can achieve stratifications on 4×4 grids in all two dimensions. Compared with such a design, the $\text{MNOA}_{\text{II}}(32, 3^5, 8, 2)$ enjoys almost the same two-dimensional space-filling property, while the newly constructed design has much more factors (15 against 9) and the column orthogonality.

3.3 Type-III MNOAs

This subsection presents a method for constructing Type-III MNOAs using the expansive replacement method. The proposed construction method is new and allows the constructed Type-III MNOAs to enjoy the attractive space-filling property and column orthogonality between groups. Note that Type-I and Type-II MNOAs are proposed by improving the within-group stratification property, while the Type-III MNOAs improve the between-group stratification property, which provide an alternative class of space-filling designs.

Definition 3 An $n \times m_1 m_2$ array with entries from $\{0, 1, \ldots, s^2 - 1\}$ is called a Type-III MNOA, denoted by $\text{MNOA}_{\text{III}}(n, {m_2}^{m_1}, s^2, p)$ with $s = \lambda_1 p^2$, where $\lambda_1 \geq 1$ is an integer, if it can be partitioned into m_1 disjoint groups each of m_2 columns, and satisfies the following properties:

(a) any two columns from different groups are column-orthogonal;
(b) any two columns from different groups achieve stratifications on $s^2 \times s$ and $s \times s^2$ grids;
(c) any two columns from the same group achieve a stratification on a $p \times p$ grid.

Compared with Definitions 1 and 2, (i) Definition 3(a) keeps the column orthogonality between groups; (ii) Definition 3(b) shows that any two columns from different groups achieve stratifications on $(\lambda_1^2 p^4) \times (\lambda_1 p^2)$ and $(\lambda_1 p^2) \times (\lambda_1^2 p^4)$ grids instead of a $(\lambda_1 p^3) \times (\lambda_1 p^3)$ grid in Definition 1(b) and a $p^2 \times p^2$ grid in Definition 2(b), respectively; (iii) Definition 3(c) shows that any two columns from the same group achieve a stratification on a $p \times p$ grid instead of $p^2 \times p$ and $p \times p^2$ grids. By Definition 3, an $\text{MNOA}_{\text{III}}(n, {m_2}^{m_1}, s^2, p)$ is a design such that any two columns form an $\text{OSOA}(n, 2, s^2, 2+)$ if they are from different groups, and can be collapsed into an $\text{OA}(n, p^2)$ if they are from the same group. Thus such a design enjoys much better space-filling property than an OA with p levels. The measure π defined in (4) can be used to evaluate the degree of both column orthogonality of Definition 3(a) and stratifications of Definition 3(b).

We now present the construction of a Type-III MNOA. The detailed construction is given by the following steps.

Construction 3

Step 1 Let X be an $\text{OA}(\lambda s^2, s^{m_1})$, where $\lambda \geq 1$ is an integer. Take A to be the $GD_{\text{I}}(X)$ and $GD_{\text{II}}(X)$ in the generalized double of X in (1), respectively.

Step 2 Based on an $\text{OA}(s, p^{m_2})$ with $s = \lambda_1 p^2$, where $\lambda_1 \geq 1$ is an integer, take B to be an $\text{LH}(s, m_2)$ obtained by, for each column, replacing the s/p entries for level j by any permutation of $js/p, js/p + 1, \ldots, (j + 1)s/p - 1$ for $j = 0, \ldots, p - 1$ (Tang 1993, OA-based Latin hypercube).

Step 3 Obtain two designs $C^{(1)}$ and $C^{(2)}$ via the expansive replacement method using the two A's and B above. According to the grouping of the columns of C in (3), write

$$C^{(k)} = (C_1^{(k)}, \ldots, C_{m_1}^{(k)}),$$

where $C_i^{(k)} = (c_{i1}^{(k)}, c_{i2}^{(k)}, \ldots, c_{im_2}^{(k)})$ for $k = 1, 2$.

Step 4 Define

$$D = sC^{(1)} + C^{(2)}, \tag{7}$$

and write $D = (D_1, \ldots, D_{m_1})$ where $D_i = (d_{i1}, d_{i2}, \ldots, d_{im_2})$ represents the ith group of m_2 columns for $i = 1, \ldots, m_1$.

For design D in (7), we have the following result.

Theorem 4 *Given an* $\mathrm{OA}(\lambda s^2, s^{m_1})$ *and an* $\mathrm{OA}(s, p^{m_2})$ *with* $s = \lambda_1 p^2$*, where* $\lambda \geq 1$ *and* $\lambda_1 \geq 1$ *are two integers, the design D in* (7) *is an* $\mathrm{MNOA}_{\mathrm{III}}(\lambda s^3, m_2{}^{m_1}, s^2, p)$.

Theorem 4 shows that Type-III MNOAs can be regarded as an extension of OSOAs of strength 2+. Specifically, an $\mathrm{MNOA}_{\mathrm{III}}(\lambda s^3, m_2{}^{m_1}, s^2, p)$ with $m_2 = 1$ becomes an $\mathrm{OSOA}(\lambda s^3, m_1, s^2, 2+)$. However, m_2 will be larger than 1 in many cases. This allows Type-III MNOAs with a considerably larger number of factors to be constructed while enjoying almost the same column orthogonality and two-dimensional stratifications as OSOAs of strength 2+.

Theorem 4 provides a series of Type-III MNOAs with the attractive space-filling properties. Sun and Tang (2017a) constructed a design in which any two columns achieve a stratification on a $p^2 \times p^2$ grid if they are from different groups, and on a $p \times p$ grid if they are from the same group, whereas, for a Type-III MNOA, any two columns from different groups achieve stratifications on $s^2 \times s$ and $s \times s^2$ grids with $s = \lambda_1 p^2$ and retain the same stratifications within a group as the design from Sun and Tang (2017a). This implies that the proposed designs have the better space-filling property. An illustrative example is as follows.

Example 6 We present the detailed steps of constructing an $\mathrm{MNOA}_{\mathrm{III}}(64, 3^5, 16, 2)$ according to Construction 3.

Step 1 Let X be an $\mathrm{OA}(16, 4^5)$. Take A to be $(X^T, X^T, X^T, X^T)^T$ and $(X^T, 1 + X^T, 2 + X^T, 3 + X^T)^T$ (modulo 4), respectively.

Step 2 Take B to be an $\mathrm{LH}(4, 3)$ obtained by, for each column of an $\mathrm{OA}(4, 2^3)$, replacing the two entries for level j by any permutation of $2j$ and $2j + 1$ for $j = 0, 1$.

Step 3 Utilizing the two A's and B above, we can generate two designs $C^{(1)}$ and $C^{(2)}$ via the expansive replacement method. According to the grouping of the columns of C in (3), write

$$C^{(1)} = (C_1^{(1)}, \ldots, C_5^{(1)}) \quad \text{and} \quad C^{(2)} = (C_1^{(2)}, \ldots, C_5^{(2)}),$$

where $C_i^{(1)} = (c_{i1}^{(1)}, c_{i2}^{(1)}, c_{i3}^{(1)})$ and $C_i^{(2)} = (c_{i1}^{(2)}, c_{i2}^{(2)}, c_{i3}^{(2)})$.

Step 4 Design $D = 4C^{(1)} + C^{(2)}$ becomes an $\mathrm{MNOA}_{\mathrm{III}}(64, 3^5, 16, 2)$, as shown in Table 8, where $D = (D_1, \ldots, D_5)$ has 5 disjoint groups of 3 columns each.

For such a design, we have that any two columns from different groups achieve stratifications on 16×4 and 4×16 grids in 90 out of 105 two dimensions, and any two columns from the same group achieve a stratification on a 2×2 grid in the remaining 15 two dimensions.

Compared with an $\mathrm{OSOA}(64, 5, 16, 2+)$ given in Zhou and Tang (2019), design D in Example 6 gains more factors (15 against 5) with almost the same column

Table 8 The $MNOA_{III}(64, 3^5, 16, 2)$ in Example 6

D_1			D_2			D_3			D_4			D_5		
0	10	15	0	10	15	0	10	15	0	10	15	0	10	15
5	5	0	0	10	15	5	5	0	5	5	0	5	5	0
10	15	5	0	10	15	10	15	5	10	15	5	10	15	5
15	0	10	0	10	15	15	0	10	15	0	10	15	0	10
0	10	15	5	5	0	5	5	0	10	15	5	15	0	10
5	5	0	5	5	0	0	10	15	15	0	10	10	15	5
10	15	5	5	5	0	15	0	10	0	10	15	5	5	0
15	0	10	5	5	0	10	15	5	5	5	0	0	10	15
0	10	15	10	15	5	10	15	5	15	0	10	5	5	0
5	5	0	10	15	5	15	0	10	10	15	5	0	10	15
10	15	5	10	15	5	0	10	15	5	5	0	15	0	10
15	0	10	10	15	5	5	5	0	0	10	15	10	15	5
0	10	15	15	0	10	15	0	10	5	5	0	10	15	5
5	5	0	15	0	10	10	15	5	0	10	15	15	0	10
10	15	5	15	0	10	5	5	0	15	0	10	0	10	15
15	0	10	15	0	10	0	10	15	10	15	5	5	5	0
1	9	12	1	9	12	1	9	12	1	9	12	1	9	12
6	7	1	1	9	12	6	7	1	6	7	1	6	7	1
11	12	6	1	9	12	11	12	6	11	12	6	11	12	6
12	2	11	1	9	12	12	2	11	12	2	11	12	2	11
1	9	12	6	7	1	6	7	1	11	12	6	12	2	11
6	7	1	6	7	1	1	9	12	12	2	11	11	12	6
11	12	6	6	7	1	12	2	11	1	9	12	6	7	1
12	2	11	6	7	1	11	12	6	6	7	1	1	9	12
1	9	12	11	12	6	11	12	6	12	2	11	6	7	1
6	7	1	11	12	6	12	2	11	11	12	6	1	9	12
11	12	6	11	12	6	1	9	12	6	7	1	12	2	11
12	2	11	11	12	6	6	7	1	1	9	12	11	12	6
1	9	12	12	2	11	12	2	11	6	7	1	11	12	6
6	7	1	12	2	11	11	12	6	1	9	12	12	2	11
11	12	6	12	2	11	6	7	1	12	2	11	1	9	12
12	2	11	12	2	11	1	9	12	11	12	6	6	7	1
2	11	13	2	11	13	2	11	13	2	11	13	2	11	13
7	4	2	2	11	13	7	4	2	7	4	2	7	4	2
8	14	7	2	11	13	8	14	7	8	14	7	8	14	7
13	1	8	2	11	13	13	1	8	13	1	8	13	1	8
2	11	13	7	4	2	7	4	2	8	14	7	13	1	8
7	4	2	7	4	2	2	11	13	13	1	8	8	14	7
8	14	7	7	4	2	13	1	8	2	11	13	7	4	2
13	1	8	7	4	2	8	14	7	7	4	2	2	11	13

Table 8 continued

D_1			D_2			D_3			D_4			D_5		
2	11	13	8	14	7	8	14	7	13	1	8	7	4	2
7	4	2	8	14	7	13	1	8	8	14	7	2	11	13
8	14	7	8	14	7	2	11	13	7	4	2	13	1	8
13	1	8	8	14	7	7	4	2	2	11	13	8	14	7
2	11	13	13	1	8	13	1	8	7	4	2	8	14	7
7	4	2	13	1	8	8	14	7	2	11	13	13	1	8
8	14	7	13	1	8	7	4	2	13	1	8	2	11	13
13	1	8	13	1	8	2	11	13	8	14	7	7	4	2
3	8	14	3	8	14	3	8	14	3	8	14	3	8	14
4	6	3	3	8	14	4	6	3	4	6	3	4	6	3
9	13	4	3	8	14	9	13	4	9	13	4	9	13	4
14	3	9	3	8	14	14	3	9	14	3	9	14	3	9
3	8	14	4	6	3	4	6	3	9	13	4	14	3	9
4	6	3	4	6	3	3	8	14	14	3	9	9	13	4
9	13	4	4	6	3	14	3	9	3	8	14	4	6	3
14	3	9	4	6	3	9	13	4	4	6	3	3	8	14
3	8	14	9	13	4	9	13	4	14	3	9	4	6	3
4	6	3	9	13	4	14	3	9	9	13	4	3	8	14
9	13	4	9	13	4	3	8	14	4	6	3	14	3	9
14	3	9	9	13	4	4	6	3	3	8	14	9	13	4
3	8	14	14	3	9	14	3	9	4	6	3	9	13	4
4	6	3	14	3	9	9	13	4	3	8	14	14	3	9
9	13	4	14	3	9	4	6	3	14	3	9	3	8	14
14	3	9	14	3	9	3	8	14	9	13	4	4	6	3

orthogonality and two-dimensional stratifications. In particular, if each group of design D has one factor, then design D becomes an OSOA(64, 5, 16, 2+). In addition, a D(64, 16^{48}) from Sun and Tang (2017a) is a design of 64 runs for 48 factors that has 8 groups each of 6 factors such that any two columns achieve a stratification on a 4×4 grid if they are from different groups, and on a 2×2 grid if they are from the same group. Compared with such a design, the D in Example 6 enjoys better space-filling property, although the former has relatively more factors. Thus, the Type-III MNOAs provide a preferable choice of designs for computer experiments.

Similar to Example 6, Table 9 lists some new Type-III MNOAs by Theorem 4 based on suitable choices of OAs for practical use.

In the rest of this section, we provide a construction of column-orthogonal Type-III MNOAs when taking B to be a column-orthogonal Latin hypercube based on an OA. This can be done as follows. Suppose that m_2 is an even integer and $s = p^2$, and let $G = (G_1, \ldots, G_{m_2/2})$ be a centered OA(s, p^{m_2}) with each G_j having two columns.

Table 9 Some Type-III MNOAs

p	$\mathrm{OA}(\lambda s^2, s^{m_1})$	$\mathrm{OA}(s, p^{m_2})$	Type-III MNOA	π
2	$\mathrm{OA}(16, 4^5)$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{III}}(64, 3^5, 16, 2)$	0.857
2	$\mathrm{OA}(32, 4^9)$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{III}}(128, 3^9, 16, 2)$	0.923
2	$\mathrm{OA}(64, 4^{21})$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{III}}(256, 3^{21}, 16, 2)$	0.968
2	$\mathrm{OA}(256, 4^{85})$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{III}}(1024, 3^{85}, 16, 2)$	0.992
2	$\mathrm{OA}(1024, 4^{341})$	$\mathrm{OA}(4, 2^3)$	$\mathrm{MNOA_{III}}(4096, 3^{341}, 16, 2)$	0.998
2	$\mathrm{OA}(64, 8^9)$	$\mathrm{OA}(8, 2^7)$	$\mathrm{MNOA_{III}}(512, 7^9, 64, 2)$	0.903
2	$\mathrm{OA}(128, 8^{17})$	$\mathrm{OA}(8, 2^7)$	$\mathrm{MNOA_{III}}(1024, 7^{17}, 64, 2)$	0.949
2	$\mathrm{OA}(512, 8^{73})$	$\mathrm{OA}(8, 2^7)$	$\mathrm{MNOA_{III}}(4096, 7^{73}, 64, 2)$	0.988
2	$\mathrm{OA}(144, 12^7)$	$\mathrm{OA}(12, 2^{11})$	$\mathrm{MNOA_{III}}(1728, 11^7, 144, 2)$	0.868
2	$\mathrm{OA}(288, 12^{12})$	$\mathrm{OA}(12, 2^{11})$	$\mathrm{MNOA_{III}}(3456, 11^{12}, 144, 2)$	0.924
2	$\mathrm{OA}(256, 16^{17})$	$\mathrm{OA}(16, 2^{15})$	$\mathrm{MNOA_{III}}(4096, 15^{17}, 256, 2)$	0.945
3	$\mathrm{OA}(81, 9^{10})$	$\mathrm{OA}(9, 3^4)$	$\mathrm{MNOA_{III}}(729, 4^{10}, 81, 3)$	0.923
3	$\mathrm{OA}(162, 9^{19})$	$\mathrm{OA}(9, 3^4)$	$\mathrm{MNOA_{III}}(1458, 4^{19}, 81, 3)$	0.960
3	$\mathrm{OA}(729, 9^{91})$	$\mathrm{OA}(9, 3^4)$	$\mathrm{MNOA_{III}}(6561, 4^{91}, 81, 3)$	0.992
4	$\mathrm{OA}(256, 16^{17})$	$\mathrm{OA}(16, 4^5)$	$\mathrm{MNOA_{III}}(4096, 5^{17}, 256, 4)$	0.952
4	$\mathrm{OA}(512, 16^{33})$	$\mathrm{OA}(16, 4^5)$	$\mathrm{MNOA_{III}}(8192, 5^{33}, 256, 4)$	0.976
5	$\mathrm{OA}(625, 25^{26})$	$\mathrm{OA}(25, 5^6)$	$\mathrm{MNOA_{III}}(15625, 6^{26}, 625, 5)$	0.968

Define $B = (G_1 V, \ldots, G_{m_2/2} V) + (p^2 - 1)/2$, where

$$V = \begin{pmatrix} p & -1 \\ 1 & p \end{pmatrix}.$$

From Lin et al. (2009), the design B is a column-orthogonal Latin hypercube with s runs and m_2 factors. Based on Construction 3 by using this design B while still using an $\mathrm{OA}(\lambda s^2, s^{m_1})$ as X, we can establish the following result.

Theorem 5 *Given an* $\mathrm{OA}(\lambda s^2, s^{m_1})$ *and an* $\mathrm{OA}(s, p^{m_2})$ *with* m_2 *being an even integer and* $s = p^2$*, a column-orthogonal* $\mathrm{MNOA_{III}}(\lambda s^3, {m_2}^{m_1}, s^2, p)$ *can be constructed from the above* X *and* B *via Construction 3.*

Theorem 5 is a special but interesting result of Theorem 4 when design B is a column-orthogonal Latin hypercube based on an OA, and it guarantees the column orthogonality of the resulting Type-III MNOAs. Similar to Table 9 and based on suitable choices of OAs, Table 10 presents some new column-orthogonal Type-III MNOAs by Theorem 5 for practical use.

Example 7 If we take an $\mathrm{OA}(81, 9^{10})$ and an $\mathrm{OA}(9, 3^4)$, we can obtain a column-orthogonal $\mathrm{MNOA_{III}}$ $(729, 4^{10}, 81, 3)$ with $\pi = 0.923$. Taking an $\mathrm{OA}(64, 4^{21})$ and an $\mathrm{OA}(4, 2^2)$ gives a column-orthogonal $\mathrm{MNOA_{III}}$ $(256, 2^{21}, 16, 2)$ with $\pi = 0.976$. Similarly, taking an $\mathrm{OA}(16, 4^5)$ and an $\mathrm{OA}(4, 2^2)$ gives a column-orthogonal

Table 10 Some column-orthogonal Type-III MNOAs

p	$\text{OA}(\lambda s^2, s^{m_1})$	$\text{OA}(s, p^{m_2})$	Type-III MNOA	π
2	$\text{OA}(16, 4^5)$	$\text{OA}(4, 2^2)$	$\text{MNOA}_{\text{III}}(64, 2^5, 16, 2)$	0.889
2	$\text{OA}(32, 4^9)$	$\text{OA}(4, 2^2)$	$\text{MNOA}_{\text{III}}(128, 2^9, 16, 2)$	0.941
2	$\text{OA}(64, 4^{21})$	$\text{OA}(4, 2^2)$	$\text{MNOA}_{\text{III}}(256, 2^{21}, 16, 2)$	0.976
2	$\text{OA}(256, 4^{85})$	$\text{OA}(4, 2^2)$	$\text{MNOA}_{\text{III}}(1024, 2^{85}, 16, 2)$	0.994
2	$\text{OA}(1024, 4^{341})$	$\text{OA}(4, 2^2)$	$\text{MNOA}_{\text{III}}(4096, 2^{341}, 16, 2)$	0.999
3	$\text{OA}(81, 9^{10})$	$\text{OA}(9, 3^4)$	$\text{MNOA}_{\text{III}}(729, 4^{10}, 81, 3)$	0.923
3	$\text{OA}(162, 9^{19})$	$\text{OA}(9, 3^4)$	$\text{MNOA}_{\text{III}}(1458, 4^{19}, 81, 3)$	0.960
3	$\text{OA}(729, 9^{91})$	$\text{OA}(9, 3^4)$	$\text{MNOA}_{\text{III}}(6561, 4^{91}, 81, 3)$	0.992
4	$\text{OA}(256, 16^{17})$	$\text{OA}(16, 4^4)$	$\text{MNOA}_{\text{III}}(4096, 4^{17}, 256, 4)$	0.955
4	$\text{OA}(512, 16^{33})$	$\text{OA}(16, 4^4)$	$\text{MNOA}_{\text{III}}(8192, 4^{33}, 256, 4)$	0.977
5	$\text{OA}(625, 25^{26})$	$\text{OA}(25, 5^6)$	$\text{MNOA}_{\text{III}}(15625, 6^{26}, 625, 5)$	0.968

$\text{MNOA}_{\text{III}}(64, 2^5, 16, 2)$ with $\pi = 0.889$. Compared with the strong group-orthogonal array SGOA(64, 20, 16, 2) (Wang et al. 2022), the column-orthogonal $\text{MNOA}_{\text{III}}(64, 2^5, 16, 2)$ achieves the comparable two-dimensional stratifications while possessing the additional property of column orthogonality, though the latter has less columns (10 against 20). So the orthogonal Type-III MNOAs can be regarded as an alternative class of space-filling designs.

4 Concluding remarks

This paper is devoted to some methods for constructing three new classes of space-filling designs (i.e., Type-I, Type-II and Type-III MNOAs) for computer experiments. These space-filling designs are constructed via the expansive replacement method based on orthogonal arrays and strong orthogonal arrays. The resulting designs enjoy attractive space-filling properties and can accommodate a large number of factors. Interestingly, the newly constructed MNOAs enjoy near or exact column orthogonality, which is also desirable for designs of computer experiments. These designs can be regarded as a marriage between mappable nearly orthogonal arrays and strong orthogonal arrays, which are very popular for computer experiments in recent developments.

Although the $\text{MNOA}_{\text{III}}(64, 3^5, 16, 2)$ has less factors than the strong group-orthogonal array SGOA(64, 20, 16, 2) (Wang et al. 2022), the proposed Type-III MNOAs tends to be useful. First, the proposed method for Type-III MNOAs is meaningful because it motivates the construction of column-orthogonal Type-III MNOAs as shown in Theorem 5, while the SGOAs are not column-orthogonal. In addition, we note that Type-I and Type-II MNOAs are proposed by improving the within-group stratification property, while the Type-III MNOAs improve the between-group stratification property, which provide an alternative class of space-filling designs. We will further study orthogonal Type-III MNOAs with much more factors in the future.

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Appendix: Proofs of theorems

Proof of Theorem 1 From Construction 1, we have that A is an OA($\lambda s^2, s^{m_1}$) and B is an LH(s, m_2) based on an SOA($s, m_2, p^2, 2+$). Due to the expansive replacement method, any two columns from the same group for D must be two columns of a repeated B up to a row permutation, implying that D satisfies Definition 1(c) according to the definition of the SOA($s, m_2, p^2, 2+$). Let (d_1, d_2) be any two columns from different groups for D. According to the expansive replacement method, (d_1, d_2) must be two columns of an OA($\lambda s^2, s^{m_1}$) up to a level permutation. Since any level permutation of an OA does not change its strength, (d_1, d_2) is an OA with s levels. Therefore, D satisfies Definitions 1(a) and 1(b). This completes the proof. □

Proof of Theorem 2 We only need to prove that the resulting design, say D, from Theorem 2 is column-orthogonal as its stratifications follow from Theorem 1. As B is column-orthogonal, then any two columns from the same group for D is column-orthogonal due to the expansive replacement method. According to the proof of Theorem 1, any two columns from different groups for D is an OA with s levels, and then is also column-orthogonal. This completes the proof. □

In order to prove Theorem 3, we first give Lemmas 1, 2 and 3. From Step 1 of Construction 2, we have the following result.

Lemma 1 (Sun and Tang 2017a) *Any four columns, derived by taking two columns from one group C_{i_1} and two columns from another group C_{i_2} with $i_1 \neq i_2$, must form an* OA($\lambda s^2, 4, p, 4$).

According to the specific structures of E and F in Step 2 of Construction 2, we have the following result.

Lemma 2 *Any three columns, derived by taking two columns from E and one column from F, must form an* OA($\lambda ps^2, 3, p, 3$).

Lemma 2 allows many three-column arrays whose columns come from E and F to have strength three, and then allows the constructed D in (6) to have the stratification property of Definition 2(c).

Note that any linear level permutation of C in Step 2 of Construction 2 does not change its strength such that $u+C$ in F has the same strength as C for $u = 1, \ldots, p-1$. From Lemma 1, a direct result is given below.

Lemma 3 *Any four columns, derived by taking two columns from one group E_{i_1} and two columns from another group F_{i_2} with $i_1 \neq i_2$, must form an* OA($\lambda ps^2, 4, p, 4$).

Lemma 3 allows many four-column arrays whose columns come from E and F to have strength four, and then allows design D in (6) to have the stratification property of Definition 2(b).

Proof of Theorem 3 From (5), we have $D^* = HR$, where $H = (H_1, \ldots, H_q)$ and $R = \text{diag}\{U, \ldots, U\}$ with U repeating q times. By Lemma 2, we see that (E, F) is an orthogonal array of strength 2, implying that H is column-orthogonal. By noting that U is also column-orthogonal, we have $D^{*T} D^* = (HR)^T HR = R^T(H^T H)R = c_1 R^T R = c_2 I_{2q}$, where c_1 and c_2 are two constants, and I_{2q} is the identity matrix of order $2q$. This shows that D^* in (5) is column-orthogonal, so is D in (6).

Before showing the stratifications of D, we first consider two mappings $h_1(x)$ and $h_2(x)$. Note that any column d of D has the following form:

$$d = bp^2 + b'p \pm b'', \tag{8}$$

where (b, b', b'') up to a column permutation is $(e_{ik}, f_{ik'}, e_{jl})$, where $k' = k + 1$ if $k \leq m_2 - 1$ and $k' = 1$ if $k = m_2$. Consider the mapping

$$h_1(x) = \left\lfloor \{x + (p^3 - 1)/2\}/p \right\rfloor - (p^2 - 1)/2 \;\; \text{with} \;\; x \in \Omega(p^3),$$

which collapses the p^3 levels in $\Omega(p^3)$ into the p^2 levels in $\Omega(p^2)$. We need to show that $h_1(d) = bp + b'$, which means that the column d becomes the column $bp + b'$ after the mapping $h_1(x)$ is applied to each entry of d. By letting $r = b + (p - 1)/2$, $r' = b' + (p - 1)/2$ and $r'' = \pm b'' + (p - 1)/2$, we have

$$\begin{aligned} h_1(d) &= \left\lfloor \{bp^2 + b'p \pm b'' + (p^3 - 1)/2\}/p \right\rfloor - (p^2 - 1)/2 \\ &= \left\lfloor (rp^2 + r'p + r'')/p \right\rfloor - (p^2 - 1)/2. \end{aligned}$$

Since all entries of $(b, b', \pm b'')$ are in $\Omega(p)$, all entries of (r, r', r'') must take values from $\{0, 1, \ldots, p - 1\}$. We then have $h_1(d) = rp + r' - (p^2 - 1)/2 = bp + b'$. We next consider the mapping

$$h_2(x) = \left\lfloor \{x + (p^3 - 1)/2\}/p^2 \right\rfloor - (p - 1)/2 \;\; \text{with} \;\; x \in \Omega(p^3),$$

which collapses the p^3 levels in $\Omega(p^3)$ into the p levels in $\Omega(p)$. By the above similar discussion, we have $h_2(d) = b$.

We now prove the stratifications of D in Definition 2(b). Consider two columns d_1 and d_2 of D as in (8), and write them as

$$d_1 = b_1 p^2 + b_1' p \pm b_1'' \quad \text{and} \quad d_2 = b_2 p^2 + b_2' p \pm b_2''.$$

Let us show that the array (d_1, d_2) can be collapsed into an OA$(\lambda ps^2, 2, p^2, 2)$, that is to say, $(h_1(d_1), h_1(d_2)) = (b_1 p + b_1', b_2 p + b_2')$ is an OA$(\lambda ps^2, 2, p^2, 2)$. In fact, this is true by noting the following two facts: (i) from Lemma 3, (b_1, b_2, b_2, b_2') is an OA($\lambda ps^2, 4, p, 4$); (ii) $p^3x_1 + p^2x_2 + px_3 + x_4$ establishes a one-to-one correspondence between the p^4 pairs (x_1, x_2, x_3, x_4) with $x_1, x_2, x_3, x_4 \in \Omega(p)$ and the p^4 levels in $\Omega(p^4)$. This shows that D satisfies Definition 2(b).

Next, we prove the stratifications of D in Definition 2(c). Let us show that the array (d_1, d_2) can be collapsed into an OA($\lambda ps^2, 2, p^2 \times p, 2$) and an OA($\lambda ps^2, 2, p \times p^2, 2$), that is to say, $(h_1(d_1), h_2(d_2)) = (b_1 p + b_1', b_2)$ and $(h_2(d_1), h_1(d_2)) = (b_1, b_2 p + b_2')$ are an OA($\lambda ps^2, 2, p^2 \times p, 2$) and an OA($\lambda ps^2, 2, p \times p^2, 2$), respectively. In fact, this is true by noting the following two facts: (i) from Lemma 2, (b_1, b_1', b_2) and (b_1, b_2, b_2') are two OA($\lambda ps^2, 3, p, 3$)'s; (ii) $px_1 + x_2$ establishes a one-to-one correspondence between the p^2 pairs (x_1, x_2) with $x_1, x_2 \in \Omega(p)$ and the p^2 levels in $\Omega(p^2)$. This shows that D satisfies Definition 2(c). This completes the proof. □

Proof of Theorem 4 From the structures of $C^{(1)}$ and $C^{(2)}$, we have that the array $(c_{kj}^{(1)}, c_{ij}^{(1)}, c_{ij}^{(2)})$ is a repeated full factorial and is hence an OA($\lambda s^3, 3, s, 3$) for any $k \neq i$. From the expansive replacement method, $c_{kl}^{(1)}$ can be obtained by permuting levels in $c_{kj}^{(1)}$ for $l \neq j$. Because of this, the array $(c_{kl}^{(1)}, c_{ij}^{(1)}, c_{ij}^{(2)})$ with $l \neq j$ is also an OA($\lambda s^3, 3, s, 3$). Then we have that the array $(c_{kl}^{(1)}, c_{ij}^{(1)}, c_{ij}^{(2)})$ has strength 3 for any $k \neq i$. According to Theorem 4 of Zhou and Tang (2019), Definitions 3(a) and 3(b) can be verified for design D in (7). Since B is an LH(s, m_2) based on an OA(s, p^{m_2}), any two columns from the same group for D can be collapsed into an OA($\lambda s^3, p^2$), implying that D satisfies Definition 3(c). This completes the proof. □

Proof of Theorem 5 We only need to prove that the resulting design, say D, from Theorem 5 is column-orthogonal as its stratifications follow from Theorem 4. From Lemma 6.27 of Hedayat et al. (1999) and the definition of X, we see that $(GD_{\mathrm{I}}(X), GD_{\mathrm{II}}(X))$ in Step 1 of Construction 3 is an OA($\lambda s^3, s^{2m_1}$). As B is column-orthogonal, then $(C^{(1)}, C^{(2)})$ is column-orthogonal according to the proof of Theorem 2, and the inner product of any two columns from the centered $(C^{(1)}, C^{(2)})$ equals zero. From (7), let (d_i, d_j) be any two columns from the centered D, then we have $d_i = sc_i^{(1)} + c_i^{(2)}$ and $d_j = sc_j^{(1)} + c_j^{(2)}$, where $c_i^{(1)}, c_i^{(2)}, c_j^{(1)}$ and $c_j^{(2)}$ are from the centered $(C^{(1)}, C^{(2)})$, implying that $d_i^T d_j = 0$ due to the column orthogonality of $(C^{(1)}, C^{(2)})$. This completes the proof. □

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