



On Construction of Mappable Nearly Orthogonal Arrays with Column-Orthogonality

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Abstract

For designs of computer experiments, two important and desirable properties are projection uniformity and column-orthogonality. However, it is always a challenging task to construct designs with both properties. This paper constructs a series of designs which possess both (near) column-orthogonality and projection uniformity, called (nearly) column-orthogonal mappable nearly orthogonal arrays (MNOAs). Furthermore, we enhance the MNOAs' projection uniformity on any one dimension by using the constructed (nearly) column-orthogonal MNOAs and rotation matrices. Compared with the existing results (such as Sun and Tang in *J Am Stat Assoc* 112:683–689, 2017), the newly constructed designs are able to accommodate more design columns and have a much better projection uniformity, for the same run sizes.

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1 Introduction

A good design for computer experiments should spread its points evenly throughout the experimental region; such a design is called a space-filling design. For designs with high dimensions, improving their lower-dimensional projection uniformity is advisable, which can decrease the variations of predictions. For example, Latin hypercube designs (LHDs) proposed by McKay, Beckman and Conover [9] can achieve the maximum stratification when projected onto any one dimension. Tang [18] constructed LHDs based on orthogonal arrays, which preserve at least a two-dimensional stratification property of orthogonal arrays. Strong orthogonal arrays proposed by He and Tang [4] and further studied by He and Tang [5] and [8], and mappable nearly orthogonal arrays (MNOAs) studied by Mukerjee, Sun and Tang [10] are both space-filling designs which enjoy the desirable low-dimensional projection uniformity properties.

Low correlation between columns is another criterion to measure the goodness of a design. Column-orthogonality can ensure that the estimates of the linear effects in a regression model can be uncorrelated. And it can also be viewed as a stepping stone to space-filling designs (Bingham, Sitter and Tang [2]). In addition, column-orthogonal space-filling designs are most useful for factor screening settings. Many efforts have been made to construct (nearly) column-orthogonal space-filling designs, see, e.g., Bingham, Sitter and Tang [2], Pang, Liu and Lin [12], Georgiou et al. [3], Wang et al. [19] and the references therein.

It is always a challenging task to construct designs with both column-orthogonality and projection uniformity. In this paper, we construct (nearly) column-orthogonal MNOAs which accommodate more columns, and enjoy relatively good projection uniformity and column-orthogonality. By using the constructed MNOAs and rotation matrices, we further obtain a new kind of space-filling designs which preserve the projection uniformity and column-orthogonality of the used MNOAs and improve the projection uniformity in one dimension, i.e., having more levels. Recently, Sun and Tang [17] have also constructed a kind of column-orthogonal space-filling designs which possess the same projection uniformity as the MNOAs. Compared to those of Sun and Tang [17], our designs have several advantages, such as enjoying more columns and better projection uniformity in many cases. For example, for designs with 64 runs, we can construct an LHD with 54 factors in which 90.57% column pairs can achieve a stratification on a 8×8 grid, while the design constructed by Sun and Tang [17] has 48 factors of 16 levels each, and only 89.36% column pairs can achieve a stratification on a 4×4 grid. Detailed comparisons with Sun and Tang [17]'s designs will be made later.

The rest of this paper is organized as follows. Relevant notation and definition are given in Sect. 2. Section 3 proposes a general construction method for ordinary MNOAs, and some methods for constructing (nearly) column-orthogonal resolvable designs with certain special structures which can be used to construct (nearly) column-orthogonal MNOAs. Section 4 uses MNOAs to construct space-filling designs with

higher levels. Further discussions and concluding remarks are given in Sect. 5. All proofs are deferred to Appendix.

2 Definitions and Notation

A design with N runs and u factors, each factor having s levels, is denoted by $D(N, s^u)$; if the s levels occur with the same frequency, it is called a balanced design; and if $s = N$, it is a Latin hypercube design (LHD), denoted by $LHD(N, u)$. A resolvable design D , denoted by $D_\lambda(N, s^u)$, is resolvable into λ parts if it can be partitioned into $D = (D_1^T, \dots, D_\lambda^T)^T$, such that each part D_w is a balanced design $D(N/\lambda, s^u)$, $w = 1, 2, \dots, \lambda$. For convenience, we assume that the s ($s \geq 2$) levels are taken to be $(-s + 1, -s + 3, \dots, s - 1)$. This paper involves with two types of orthogonality: (i) combinatorial-orthogonality and (ii) column-orthogonality. A $D(N, s^u)$ is called an orthogonal array of strength t , denoted by $OA(N, u, s, t)$, if for each $N \times t$ submatrix, all possible level combinations occur with the same frequency. This orthogonality is called the combinatorial-orthogonality, which can lead to t - and lower-dimensional projection uniformity properties. Another orthogonality is the column-orthogonality, which means that the inner product between any two columns of a design is zero, and such a design is called a column-orthogonal design. For a design with centered levels, if it can achieve combinatorial-orthogonality, then it must be column-orthogonal.

When neither combinatorial-orthogonality nor column-orthogonality is possible, we will consider the near orthogonality. Sun and Tang [10] proposed a new class of nearly orthogonal arrays which achieve near combinatorial-orthogonality, called mappable nearly orthogonal arrays (MNOAs). The definition of MNOA in Sun and Tang [10] is based on nonnegative levels. Below we restate it with a slight modification to suit for designs with centered levels.

Definition 2.1 An $N \times um$ array with entries from set $\{-(s - 1), -(s - 3), \dots, s - 1\}$ is called a mappable nearly orthogonal array (MNOA), denoted by $MNOA(N; (s^u)^m, (p^u)^m)$, if it can be divided into m disjoint groups each having u columns, and satisfies the following properties:

- (i) any two columns from different groups achieve combinatorial-orthogonality based on s levels;
- (ii) the whole array can be mapped into an $OA(N, um, p, 2)$, where the mapping rule is that each level from interval $[-s + 2(j - 1)v, -s + 2jv]$ maps to level $-p + 2j - 1$, where $s = vp$, $j = 1, 2, \dots, p$.

This definition implies that any two columns from different groups can achieve a stratification on an $s \times s$ grid, and any two distinct columns from the same group can achieve a stratification on a $p \times p$ grid. This attractive space-filling property is very useful in computer experiments. Mukerjee, Sun and Tang [10] used the ratio of column pairs that can achieve a stratification on an $s \times s$ grid to measure the degree of combinatorial-orthogonality of an MNOA, that is,

$$\pi = u^2 \binom{m}{2} / \binom{mu}{2} = (m - 1)u / (mu - 1). \tag{2.1}$$

It is easy to see that π strictly decreases with u , and increases with m . Then $\pi \geq 4u/(5u - 1) > 80\%$ for $m \geq 5$, which implies that the MNOA with $m \geq 5$ has relatively better combinatorial-orthogonality and projection uniformity.

For a design $D = (d_1, d_2, \dots, d_u)_{n \times u}$, denote

$$\rho_{ij}(D) = \frac{d_i^T d_j}{\sqrt{d_i^T d_i} \sqrt{d_j^T d_j}} \text{ and } \rho(D) = (\rho_{ij}(D))_{u \times u}, \tag{2.2}$$

where d_i is the i th column of D . If design D has centered levels, $\rho_{ij}(D)$ is the correlation coefficient between the i th and j th columns of D . A design with small correlations is called a nearly column-orthogonal design. Two commonly used measures of near column-orthogonality are $\rho^2(D) = \sum_{i < j} 2\rho_{ij}^2(D)/(m(m - 1))$ and $\rho_M(D) = \max_{i < j} |\rho_{ij}(D)|$.

Remark 2.2 Throughout this paper, a (nearly) column-orthogonal design means that this design is at least nearly column-orthogonal; it is either nearly column-orthogonal or exactly column-orthogonal.

3 Construction of MNOAs

In this section, we first provide a general construction method for MNOAs, using a special resolvable design and an orthogonal array, and then construct such special (nearly) column-orthogonal resolvable designs for three cases which can be used to construct (nearly) column-orthogonal MNOAs.

3.1 General Construction of MNOAs

Algorithm 3.1 (Construction of MNOAs)

- Step 1. Let $D = (D_1^T, \dots, D_\lambda^T)^T$ be a resolvable design $D_\lambda(\lambda s, s^u)$ that can be mapped into an $OA(\lambda s, u, p, 2)$, where $s = vp$ and v is a positive integer. Let $d_w(j)$ denote the j th row of D_w , where $w = 1, 2, \dots, \lambda$, and $j = 1, 2, \dots, s$.
- Step 2. Let $B = (b_{ij})$ be an $OA(n, m, s, 2)$.
- Step 3. Construct a matrix A_j^w of order $n \times u$ with the i th row being $d_w((b_{ij} + s + 1)/2)$ for $1 \leq i \leq n, 1 \leq j \leq m$.
- Step 4. Juxtapose matrices $A_j^1, A_j^2, \dots, A_j^\lambda$ row by row to obtain a $\lambda n \times u$ matrix $A_j = (A_j^{1T}, A_j^{2T}, \dots, A_j^{\lambda T})^T$.
- Step 5. Juxtapose matrices A_1, A_2, \dots, A_m column by column to obtain design $A = (A_1, A_2, \dots, A_m)$ of order $\lambda n \times um$.

Theorem 3.2 *If there exists an $OA(n, m, s, 2)$, denoted by B , and a resolvable design $D_\lambda(\lambda s, s^u)$, denoted by D that can be mapped into an $OA(\lambda s, u, p, 2)$, then the matrix $A = (A_1, A_2, \dots, A_m)$ constructed through Algorithm 3.1 is an MNOA($\lambda n; (s^u)^m, (p^u)^m$), and the correlation matrix of A is $\rho(A) = I_m \otimes \rho(D)$, specially $\rho(A) = I_{um}$ when $\rho(D) = I_u$.*

From Theorem 3.2, the column-orthogonality of the constructed MNOA is determined by design D . That is, if we take D to be a (nearly) column-orthogonal design, then the constructed design A is a (nearly) column-orthogonal MNOA. Next we consider the construction of resolvable designs that are needed for obtaining (nearly) column-orthogonal MNOAs.

3.2 (Nearly) Column-Orthogonal Resolvable Designs Based on Orthogonal Arrays

For the construction of a (nearly) column-orthogonal resolvable design $D_\lambda(\lambda s, s^u)$ that can be mapped into an $OA(\lambda s, u, p, 2)$, we just consider the following three cases with $\alpha \geq 2$ being a positive integer: (1) $s = p^\alpha$ and $\lambda = 1$; (2) $s = p^\alpha$ and $\lambda = p$; and (3) $s = kp^\alpha$ with k being a positive integer and $\lambda = 1$ or p .

3.2.1 Case of $s = p^\alpha$ and $\lambda = 1$

Since $\lambda = 1$, only a (nearly) column-orthogonal LHD(s, u) is needed to be mapped into an $OA(s, u, p, 2)$.

Denote rotation matrices R_d^p for $d = 1, 2, \dots$ as follows (with $R_0^p = 1$)

$$R_d^p = \begin{pmatrix} p^{2^{d-1}} R_{d-1}^p & -R_{d-1}^p \\ R_{d-1}^p & p^{2^{d-1}} R_{d-1}^p \end{pmatrix} \text{ and } R_{u,d}^p = \text{diag}\{R_d^p, R_d^p, \dots, R_d^p\}, \quad (3.1)$$

where u is a multiple of 2^d and R_d^p occurs $u/2^d$ times in $R_{u,d}^p$. From (3.1), we know that R_d^p is a $2^d \times 2^d$ matrix which comprises of columns of permutation of $\{1, p, \dots, p^{2^d-1}\}$ (up to sign changes) with $(R_d^p)^T R_d^p = \frac{p^{2^{d+1}}-1}{p^2-1} I_{2^d}$, and then, $(R_{u,d}^p)^T R_{u,d}^p = \frac{p^{2^{d+1}}-1}{p^2-1} I_u$.

Let $T_{u,\alpha,t}^p = \text{diag}\{T_{\alpha,t}^p, T_{\alpha,t}^p, \dots, T_{\alpha,t}^p\}$, where $T_{\alpha,t}^p$ is an $\alpha \times t$ matrix which comprises of columns of permutation of $\{1, p, \dots, p^{\alpha-1}\}$ (up to sign changes), u is a multiple of t , and $T_{\alpha,t}^p$ occurs u/t times in $T_{u,\alpha,t}^p$.

Then a result in Sun, Pang and Liu [16] can be applied.

Lemma 3.3 (Sun, Pang and Liu [16]) *Suppose C is an $OA(p^\alpha, c, p, 2)$ with $c = v\alpha$, in which the i th group of α consecutive columns compose a full factorial design, $i = 1, 2, \dots, v$. Then*

- (i) for $\alpha = 2^d$, $D = CR_{u,d}^p$ is a column-orthogonal LHD(p^α, u) with $u = c$;
- (ii) for $\alpha \neq 2^d$, $D = CT_{u,\alpha,t}^p$ is an LHD(p^α, u) with $u = vt$ and $\rho(D) = \rho(T_{u,\alpha,t}^p)$.

Lemma 3.3 involves the methods of partitioning the $OA(p^\alpha, c, p, 2)$ into v parts with each part being a full factorial design of α factors (see Steinberg and Lin [14], Pang, Liu and Lin [12], and Ai, He and Liu [1] for the details).

Let $(G_1, G_2, \dots, G_\alpha)$ be a full factorial design $D(p^\alpha, p^\alpha)$. Obviously, the levels of $G_{i_1}(\pm p^0) + G_{i_2}(\pm p^1) + \dots + G_{i_\alpha}(\pm p^{\alpha-1})$ are a permutation of $-p^\alpha + 1, -p^\alpha + 3, \dots, p^\alpha - 1$, where $(i_1, i_2, \dots, i_\alpha)$ is a permutation of $(1, 2, \dots, \alpha)$. It is clear that if

Table 1 Some (nearly) column-orthogonal MNOAs for the case of $s = p^\alpha$ and $\lambda = 1$

p	α	B	C	MNOA	π
2	2	OA(16, 5, 4, 2)	OA(4, 2, 2, 2)	MNOA(16; $(4^2)^5, (2^2)^5$)	0.8889
2	3	OA(64, 9, 8, 2)	OA(8, 6, 2, 2)	MNOA(64; $(8^6)^9, (2^6)^9$)*	0.9057
2	4	OA(256, 17, 16, 2)	OA(16, 12, 2, 2)	MNOA(256; $(16^{12})^{17}, (2^{12})^{17}$)	0.9458
3	2	OA(81, 10, 9, 2)	OA(9, 4, 3, 2)	MNOA(81; $(9^4)^{10}, (3^4)^{10}$)	0.9231
4	2	OA(256, 17, 16, 2)	OA(16, 4, 4, 2)	MNOA(256; $(16^4)^{17}, (4^4)^{17}$)	0.9552
5	2	OA(625, 26, 25, 2)	OA(25, 6, 5, 2)	MNOA(625; $(25^6)^{26}, (5^6)^{26}$)	0.9677

B is the design in Theorem 3.2 and C is the design in Lemma 3.3 that can be used to construct the design D in Theorem 3.2, π is the ratio given in (2.1). All the designs are column-orthogonal except that the design marked with “*” is nearly column-orthogonal

$G_{i_1}(\pm p^0) + G_{i_2}(\pm p^1) + \dots + G_{i_\alpha}(\pm p^{\alpha-1})$ is mapped to p levels, it becomes $\pm G_{i_\alpha}$. Then if $(G_{i_1}(\pm p^0) + G_{i_2}(\pm p^1) + \dots + G_{i_\alpha}(\pm p^{\alpha-1}), G_{j_1}(\pm p^0) + G_{j_2}(\pm p^1) + \dots + G_{j_\alpha}(\pm p^{\alpha-1}))$ can be mapped into an OA($p^\alpha, 2, p, 2$), one only needs that $(G_{i_\alpha}, G_{j_\alpha})$ is an OA($p^\alpha, 2, p, 2$). The following theorem can be established.

Theorem 3.4 For the designs constructed in Lemma 3.3,

- (i) when $\alpha = 2^d$, the design LHD(p^α, u) can be mapped into an OA($p^\alpha, u, p, 2$);
- (ii) when $\alpha \neq 2^d$, if the t entries of $\pm p^{\alpha-1}$ in $T_{\alpha,t}^p$ are in different rows of $T_{\alpha,t}^p$, then the design LHD(p^α, u) can be mapped into an OA($p^\alpha, u, p, 2$).

Theorems 3.2 and 3.4 and Lemma 3.3 can be used to construct (nearly) column-orthogonal MNOA($n; (s^u)^m, (p^u)^m$)’s with $s = p^\alpha$. In particular, the resulting MNOAs can achieve exact column-orthogonality when $\alpha = 2^d$. We summarize some MNOAs for the case of $s = p^\alpha$ in Table 1. As the ratio π in (2.1) increases with m , we take the saturated OA($s^2, s + 1, s, 2$) as design B for $s = p^\alpha$ being a prime power to get a larger π and make the constructed design be comparable to that of Mukerjee, Sun and Tang [10]. Here $m = s + 1 = p^\alpha + 1 \geq 5$, and then $\pi > 0.8$, that is a good two-dimensional stratification property can be guaranteed. The u ’s in the constructed MNOAs are usually a little smaller than those of the ordinary MNOAs, as the resolvable design D here enjoys much better column-orthogonality. So there are some MNOAs in Table 1 which have less columns than those of Series 1 in Table 2 of Mukerjee, Sun and Tang [10], but the designs in Table 1 can achieve column-orthogonality except that the MNOA with $(p, \alpha) = (2, 3)$ achieves near column-orthogonality. In addition, both the nearly column-orthogonal MNOA and exactly column-orthogonal MNOA for $(p, \alpha) = (2, 3)$ are shown in Example 3.5.

Example 3.5 Suppose B is an OA(64, 9, 8, 2), C is an OA(8, 6, 2, 2) in which every three consecutive columns in the order compose a full factorial design, and let

$$T_{3,3}^2 = \begin{pmatrix} 1 & -4 & 2 \\ 2 & -1 & -4 \\ 4 & 2 & 1 \end{pmatrix}.$$

Table 2 OA(8, 6, 2, 2) and LHD(8, 6) in Example 3.5

C: OA(8, 6, 2, 2)						D: LHD(8, 6)					
-1	-1	-1	-1	-1	-1	-7	3	1	-7	3	1
1	-1	-1	1	-1	1	-5	-5	5	3	-1	7
1	1	-1	-1	1	-1	-1	-7	-3	-3	1	-7
1	1	1	-1	-1	1	7	-3	-1	1	7	3
-1	1	1	1	-1	-1	5	5	-5	-5	-5	5
1	-1	1	1	1	-1	3	-1	7	-1	-7	-3
-1	1	-1	1	1	1	-3	1	-7	7	-3	-1
-1	-1	1	-1	1	1	1	7	3	5	5	-5

From Lemma 3.3 and Theorem 3.4, $D = CT_{6,3,3}^2$ is an LHD(8, 6), and it can be mapped into an OA(8, 6, 2, 2) that is any two columns of this LHD(8, 6) can achieve a stratification on a 2×2 grid. The matrices C and D are shown in Table 2. It is easy to calculate that $\rho_M(D) = \rho_M(T_{6,3,3}^2) = 0.0952$, and $\rho^2(D) = \rho^2(T_{6,3,3}^2) = 0.0036$. Then from Lemma 3.3, D is a nearly column-orthogonal LHD(8, 6). By Theorem 3.2, using B and D , we can obtain a nearly column-orthogonal MNOA(64; $(8^6)^9, (2^6)^9$), denoted by A , and $\rho(A) = I_9 \otimes \rho(D)$ with $\rho_M(A) = \rho_M(D) = 0.0952$. In addition, the design

$$\begin{pmatrix} 1 & 3 & 5 & 7 & -1 & -3 & -5 & -7 \\ 3 & -1 & 7 & -5 & -3 & 1 & -7 & 5 \\ 5 & -7 & -1 & 3 & -5 & 7 & 1 & -3 \\ 7 & 5 & -3 & -1 & -7 & -5 & 3 & 1 \end{pmatrix}^T,$$

constructed by Sun, Liu and Lin [15], is a column-orthogonal LHD(8, 4), and it can be mapped into an OA(8, 4, 2, 2). Consequently, it can be used, along with B , to construct a column-orthogonal MNOA(64; $(8^4)^9, (2^4)^9$).

3.2.2 Case of $s = p^\alpha$ and $\lambda = p$

For this case, we construct a (nearly) column-orthogonal resolvable design $D_p(p^{\alpha+1}, s^u)$, which can be mapped into an OA($p^{\alpha+1}, u, p, 2$). Here we need a difference scheme $D(r, c, s)$, which is an $r \times c$ array with s entries from a finite Abelian group $\{0, 1, \dots, s-1\}$ with a binary operation $+_b$ such that every element of $\{0, 1, \dots, s-1\}$ in the vector difference between any two columns of the array appears equally often.

Now in order to construct the design we need, we first produce a special matrix G :

$$G = 2 \left(E \oplus_b \frac{F + (p-1)J_{p^\alpha \times f}}{2} \right) - (p-1)J_{p^{\alpha+1} \times ef}, \tag{3.2}$$

where E is a difference scheme $D(p, e, p)$, F is an OA($p^\alpha, f, p, 2$), $J_{a \times b}$ denotes an $a \times b$ matrix with all entries one, and for two matrices $A = (a_{ij})_{m \times k}$ and $B = (b_{ij})_{n \times l}$,

their Kronecker sum “ \oplus_b ” based on $+_b$ is defined as

$$A \oplus_b B = (a_{ij} +_b B)_{mn \times kl}.$$

Note that the operation $(F + (p - 1)J_{p^\alpha \times f})/2$ is aimed at transforming the levels of F from $\{-p+1, -p+3, \dots, p-1\}$ to $\{0, 1, \dots, p-1\}$ so that the operation \oplus_b between F and the difference scheme E can be performed. And G is an $OA(p^{\alpha+1}, ef, p, 2)$.

The theorem below shows how to use matrix G to construct the design $D_p(p^{\alpha+1}, s^u)$ that can be mapped into an $OA(p^{\alpha+1}, u, p, 2)$.

Theorem 3.6 *Suppose G is defined in (3.2), F is an $OA(p^\alpha, f, p, 2)$ with $\alpha \geq 2$, and when $\alpha \geq 3$, $f = v\alpha$ and its i th consecutive α columns compose a full factorial design for all $i = 1, 2, \dots, v$. Then*

- (i) *if $\alpha = 2$ and $ef = 2l + r$ with $r = 0$ or 1 , then $D = G \begin{pmatrix} R_{2l,1}^p \\ 0_{r \times 2l} \end{pmatrix}$ is a column-orthogonal resolvable $D_p(p^3, s^u)$ that can be mapped into an $OA(p^3, u, p, 2)$, where $u = 2l$;*
- (ii) *if $\alpha = 2^d$ with $d \geq 2$, then $D = GR_{u,d}^p$ is a column-orthogonal resolvable $D_p(p^{\alpha+1}, s^u)$ that can be mapped into an $OA(p^{\alpha+1}, u, p, 2)$, where $u = ef = ev\alpha$;*
- (iii) *if $\alpha \neq 2^d$, and the t entries of $\pm p^{\alpha-1}$ in $T_{\alpha,t}^p$ are in different rows of $T_{\alpha,t}^p$, then $D = GT_{u,\alpha,t}^p$ is a resolvable $D_p(p^{\alpha+1}, s^u)$ that can be mapped into an $OA(p^{\alpha+1}, u, p, 2)$ with $\rho(D) = \rho(T_{u,\alpha,t}^p)$, where $u = evt$.*

Next, let us see two illustrative examples.

Example 3.7 Suppose E is a $D(2, 2, 2)$ with

$$E = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

and F is an $OA(8, 6, 2, 2)$. From (3.2), matrix $G = 2(E \oplus_b (F + J_{8 \times 6})/2) - J_{16 \times 12}$ is an $OA(16, 12, 2, 2)$. Now, take

$$T_{3,3}^2 = \begin{pmatrix} 1 & -4 & 2 \\ 2 & -1 & -4 \\ 4 & 2 & 1 \end{pmatrix}.$$

Theorem 3.6(iii) implies that $D = GT_{12,3,3}^2$ is a nearly column-orthogonal $D_2(16, 8^{12})$ which can be mapped into an $OA(16, 12, 2, 2)$ with $\rho_M(D) = \rho_M(T_{12,3,3}^2) = 0.0952$. Matrices G and D are given in Table 3. Now let B be an $OA(64, 9, 8, 2)$, using Theorem 3.2, B and D , a nearly column-orthogonal MNOA(128; $(8^{12})^9, (2^{12})^9$), denoted by A , can be obtained. Moreover, we have $\rho_M(A) = \rho_M(D) = 0.0952$.

Example 3.8 Let F be an $OA(4, 3, 2, 2)$ and E be a $D(2, 2, 2)$ as follows,

$$F = \begin{pmatrix} -1 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \text{ and } E = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Matrix $G = 2(E \oplus_b (F + J_{4 \times 3})/2) - J_{8 \times 6}$ can be obtained via Eq. (3.2). Following Theorem 3.6(i) with G and $R_{6,1}^2$, a column-orthogonal resolvable $D_2(8, 4^6) = GR_{6,1}^2$ can be constructed as follows,

$$D_2(8, 4^6) = \begin{pmatrix} -1 & 3 & -1 & 3 & -1 & 3 \\ 1 & -3 & -3 & -1 & 3 & 1 \\ -3 & -1 & 3 & 1 & 1 & -3 \\ 3 & 1 & 1 & -3 & -3 & -1 \\ -1 & 3 & -3 & -1 & 1 & -3 \\ 1 & -3 & -1 & 3 & -3 & -1 \\ -3 & -1 & 1 & -3 & -1 & 3 \\ 3 & 1 & 3 & 1 & 3 & 1 \end{pmatrix}.$$

Next taking an $OA(16, 5, 4, 2)$ and $D_2(8, 4^6)$, a column-orthogonal MNOA($32; (4^6)^5, (2^6)^5$) can be constructed, as shown in Table 4. Owing to the resolvable property of $D_2(8, 4^6)$, the constructed design MNOA($32; (4^6)^5, (2^6)^5$) also is a resolvable design $D_2(32, 4^{30})$.

Here we wish that the constructed MNOAs have as many columns as possible while keeping the column-orthogonality and combinatorial-orthogonality. According to Theorem 6.6 of Hedayat, Sloane and Stufken [6], there always exists a difference scheme $D(p, p, p)$ for any prime p . Then take $D(p, p, p)$ as design E , and the saturated $OA(s^2, s + 1, s, 2)$ as design B , the constructed MNOA($ps^2; (s^u)^{s+1}, (p^u)^{s+1}$)’s having much more columns are listed in Table 5 for the case of $s = p^\alpha$ and $\lambda = p$. The MNOAs with ps^2 runs can also be constructed by using $OA(ps^2, m, s, 2)$ and LHD(s, u) in Sect. 3.2.1, but the resulting MNOAs always have less columns than those constructed here.

Remark 3.9 When λ is neither 1 nor p , we cannot construct an MNOA with more columns than that of $\lambda = 1$ so far, and thus will take no account of these cases.

3.2.3 Case of $s = kp^\alpha$ and $\lambda = 1$ or p

Let $H = (h_{ij})_{k \times u}$ be an LHD(k, u), and $L_i = (L_{i1}, \dots, L_{iu})$ be an LHD(w, u), where L_{ij} is the j th column of $L_i, i = 1, \dots, k, j = 1, \dots, u$. Take

$$D_i = (kL_{i1} + h_{i1}, kL_{i2} + h_{i2}, \dots, kL_{iu} + h_{iu}), \quad i = 1, \dots, k, \text{ and} \quad (3.3)$$

$$D = (D_1^T, \dots, D_k^T)^T. \quad (3.4)$$

The following result, from Huang, Yang and Liu [7], can be applied.

Table 4 Column-orthogonal MNOA(32; $(4^6)^5, (2^6)^5$) in Example 3.8

MNOA(32; $(4^6)^5, (2^6)^5$)																																						
-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3			
-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	
-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	
-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	
1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	
1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	
1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	
1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	
1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	
-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	
-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	
-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	
3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1
3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1
3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1
3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1	-3	-3	-1	3	1	1

Table 5 Some (nearly) column-orthogonal MNOAs for the case of $s = p^\alpha$ and $\lambda = p$

p	α	B	F	MNOA	π
2	2	OA(16, 5, 4, 2)	OA(4, 3, 2, 2)	MNOA(32; $(4^6)^5, (2^6)^5$)	0.8276
2	3	OA(64, 9, 8, 2)	OA(8, 6, 2, 2)	MNOA(128; $(8^{12})^9, (2^{12})^9$)*	0.8972
2	4	OA(256, 17, 16, 2)	OA(16, 12, 2, 2)	MNOA(512; $(16^{24})^{17}, (2^{24})^{17}$)	0.9435
3	2	OA(81, 10, 9, 2)	OA(9, 4, 3, 2)	MNOA(243; $(9^{12})^{10}, (3^{12})^{10}$)	0.9076
4	2	OA(256, 17, 16, 2)	OA(16, 5, 4, 2)	MNOA(1024; $(16^{20})^{17}, (4^{20})^{17}$)	0.9440

B is the design in Theorem 3.2, and F is the design in Theorem 3.6 that can be used to construct the design D in Theorem 3.2, π is the ratio given in (2.1). All the designs are column-orthogonal except that the design marked with “*” is nearly column-orthogonal

Lemma 3.10 (Huang, Yang and Liu [7]) *The design D in (3.4) is an LHD(kw, u) with*

$$\rho_{ij}(D) = (1 - \theta)(\rho_{ij}(L_1) + \dots + \rho_{ij}(L_k))/k + \theta\rho_{ij}(H) \tag{3.5}$$

for $1 \leq i < j \leq u$, where $\theta = (k^2 - 1)/(w^2k^2 - 1)$.

We first consider the case of $\lambda = 1$. Based on the above lemma, we can construct an LHD(kp^α, u) that can be mapped into an OA($kp^\alpha, u, p, 2$) and its correlation matrix can be found by (3.5) for $w = p^\alpha$.

Theorem 3.11 *If the design L_i can be mapped into an OA($w, u, p, 2$), then the design D in (3.4) can be mapped into an OA($kw, u, p, 2$). Furthermore, when $w = p^\alpha$ and L_i is constructed in Theorem 3.4, we have*

- (i) for $\alpha = 2^d$, D is (nearly) column-orthogonal with $|\rho_{ij}(D)| < 1/16$. Specially, D is column-orthogonal when H is column-orthogonal;
- (ii) for $\alpha \neq 2^d$, let $L_i = C_i T_{u,\alpha,t}$ with C_i being an OA($p^\alpha, c, p, 2$), then $|\rho_{ij}(D)| \leq |\rho_{ij}(T_{u,\alpha,t})| + 1/64$.

For the case of $s = kp^\alpha$ and $\lambda = p$, combining Theorems 3.6 and 3.11, we can construct the resolvable design $D_p(ps, s^u)$ which can be mapped into an OA($ps, u, p, 2$). The following example illustrates the construction for the case of $\lambda = 1$.

Example 3.12 Let $p = 3, \alpha = 2$ and $k = 2$. Suppose C_1 is an OA(9, 4, 3, 2), where

$$C_1 = \begin{pmatrix} -2 & -2 & -2 & 0 & 0 & 0 & 2 & 2 & 2 \\ -2 & 0 & 2 & -2 & 0 & 2 & -2 & 0 & 2 \\ -2 & 0 & 2 & 2 & -2 & 0 & 0 & 2 & -2 \\ -2 & 0 & 2 & 0 & 2 & -2 & 2 & -2 & 0 \end{pmatrix}^T$$

and C_2 is obtained by permuting the columns of C_1 in the order of (3, 1, 4, 2). Let $R_1^3 = \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix}$. Then $L_1 = C_1 R_{4,1}^3$ and $L_2 = C_2 R_{4,1}^3$ are both a column-orthogonal LHD(9, 4), where

$$(L_1^T, L_2^T)^T = \begin{pmatrix} -8 & -6 & -4 & -2 & 0 & 2 & 4 & 6 & 8 & -8 & -2 & 4 & 6 & -6 & 0 & 2 & 8 & -4 \\ -4 & 2 & 8 & -6 & 0 & 6 & -8 & -2 & 4 & -4 & -6 & -8 & -2 & 2 & 0 & 6 & 4 & 8 \\ -8 & 0 & 8 & 6 & -4 & -2 & 2 & 4 & -6 & -8 & 0 & 8 & -2 & 6 & -4 & 4 & -6 & 2 \\ -4 & 0 & 4 & -2 & 8 & -6 & 6 & -8 & 2 & -4 & 0 & 4 & -6 & -2 & 8 & -8 & 2 & 6 \end{pmatrix}^T$$

Next, take $H = \begin{pmatrix} -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix}$. From (3.3), we have

$$D = \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} = \begin{pmatrix} -17 & -13 & -9 & -5 & -1 & 3 & 7 & 11 & 15 & -15 & -3 & 9 & 13 & -11 & 1 & 5 & 17 & -7 \\ -7 & 5 & 17 & -11 & 1 & 13 & -15 & -3 & 9 & -9 & -13 & -17 & -5 & 3 & -1 & 11 & 7 & 15 \\ -17 & -1 & 15 & 11 & -9 & -5 & 3 & 7 & -13 & -15 & 1 & 17 & -3 & 13 & -7 & 9 & -11 & 5 \\ -7 & 1 & 9 & -3 & 17 & -11 & 13 & -15 & 5 & -9 & -1 & 7 & -13 & -5 & 15 & -17 & 3 & 11 \end{pmatrix}^T$$

Note that D is a nearly column-orthogonal LHD(18, 4) with

$$\rho_{ij}(D) = \frac{k^2 - 1}{k^2 p^{2\alpha} - 1} \rho_{ij}(H) = \frac{3}{323} \rho_{ij}(H) = 0.0093 \rho_{ij}(H) \text{ for } i \neq j,$$

that is,

$$\rho(D) = \begin{pmatrix} 1 & -0.0093 & 0.0093 & -0.0093 \\ -0.0093 & 1 & -0.0093 & 0.0093 \\ 0.0093 & -0.0093 & 1 & -0.0093 \\ -0.0093 & 0.0093 & -0.0093 & 1 \end{pmatrix}.$$

When D is mapped to three levels, it becomes $C = (C_1^T, C_2^T)^T$. Let B be an OA(648, 18, 18, 2), a nearly column-orthogonal MNOA(648; $(18^4)^{18}, (3^4)^{18}$) can be constructed by Theorem 3.2.

4 Designs with High Levels

Several references have focused on the construction of column-orthogonal space-filling designs through orthogonal arrays and rotation matrices, see, e.g., Sun, Pang and Liu [16], Ai, He and Liu [1] and [19]. Inspired by this traditional thinking, in this section, we will construct some column-orthogonal space-filling designs with much better projection uniformity, through MNOAs and rotation matrices. The resulting designs improve the one-dimensional projection uniformity of the used MNOAs.

Now let $D(N, s^{um}; (q^u)^m, (p^u)^m)$ denote a $D(N, s^{um})$ with the same projection uniformity as that of an MNOA($N; (q^u)^m, (p^u)^m$), and $LHD(N, um; (q^u)^m, (p^u)^m)$ is defined similarly. We then extend these two definitions to the case that the groups may have different numbers of columns. Let $D(N, s^{\sum_{i=1}^r u_i m_i}; (q^{u_1})^{m_1} \dots (q^{u_r})^{m_r}, (p^{u_1})^{m_1} \dots (p^{u_r})^{m_r})$ denote a $D(N, s^{\sum_{i=1}^r u_i m_i})$ which can be partitioned into $\sum_{i=1}^r m_i$ groups with m_i groups each having u_i columns such that any two columns from different groups can achieve a stratification on a $q \times q$ grid, and any two distinct columns from the whole design can achieve a stratification on a $p \times p$ grid, and $LHD(N, \sum_{i=1}^r u_i m_i; (q^{u_1})^{m_1} \dots (q^{u_r})^{m_r}, (p^{u_1})^{m_1} \dots (p^{u_r})^{m_r})$ is defined similarly.

Algorithm 4.1 (Construction of designs with more levels)

- Step 1. Suppose $A = (A_1, A_2, \dots, A_m)$ is an MNOA($\lambda n; (s^u)^m, (p^u)^m$), where A_i is a matrix of order $\lambda n \times u$ with $i = 1, 2, \dots, m$.
- Step 2. For $i = 1, 2, \dots, u$, set $P_i = (A_{1i}, A_{2i}, \dots, A_{mi})$, where A_{ji} denotes the i th column of A_j , then P_i is an OA($\lambda n, m, s, 2$).
- Step 3. Suppose $um = a + r$ with $a = 2l$ and $r = 0$ or 1 , then take

$$K = (P_1, P_2, \dots, P_u) \begin{pmatrix} R_{a,1}^s \\ 0_{r \times a} \end{pmatrix}.$$

Partition K as $K = (K_1, K_2, \dots, K_u)$, where K_i is a matrix of order $\lambda n \times m$ with $i = 1, 2, \dots, u - 1$, and K_u is a matrix of order $\lambda n \times (m - r)$.

Step 4. Let $L_i = (K_{1i}, \dots, K_{ui})$ with $i = 1, 2, \dots, m - 1$, and $L_m = (K_{1m}, \dots, K_{(u-r)m})$, where K_{ji} is the i th column of K_j .

Step 5. Let $L = (L_1, \dots, L_m)$.

Theorem 4.2 *The design L constructed by Algorithm 4.1 is a $D(\lambda n, (s^2)^{um-r}; (s^u)^{m-1} (s^{u-r})^1, (p^u)^{m-1} (p^{u-r})^1)$. Furthermore, if A is constructed by Algorithm 3.1 with $\rho(A) = I_m \otimes \rho(D)$, then*

- (i) L is column-orthogonal when $\rho(D) = I_u$;
- (ii) $\rho(L) = \rho(A) = I_m \otimes \rho(D)$ when m is even;
- (iii) $|\rho_{ij}(L)| \leq \rho_M(D)$ when m is odd with $i, j = 1, 2, \dots, um - r$ and $i \neq j$.

The constructed designs in Theorem 4.2 preserve the stratification properties and column-orthogonality of A , and they usually have more columns or better projection uniformity than that of Sun, Pang and Liu [16] for the same run sizes and numbers of levels. Compared to the designs constructed in Ai, He and Liu [1], the constructed designs in Theorem 4.2 can achieve much better projection uniformity. An illustrative example is as follows.

Example 4.3 Using the column-orthogonal MNOA(81; $(9^4)^{10}, (3^4)^{10}$) in Table 1, a column-orthogonal LHD(81, 40; $(9^4)^{10}, (3^4)^{10}$), denoted by D_1 , can be constructed. Any two columns from different groups of D_1 can achieve a stratification on a 9×9 grid, and any two distinct columns from the whole design can achieve a stratification on a 3×3 grid. Let A be an OA(81, 40, 3, 2) which is a three-level regular saturated design of strength two and 81 runs. Using the method in Sun, Pang and Liu [16], a column-orthogonal LHD(81, 40), $D_2 = AR_{40,2}^3$, can be constructed, which achieves a stratification on a 3×3 grid in any two dimensions. D_2 also has some pairs of columns that can achieve a stratification on a 9×9 grid, but the number of such pairs is less than that of D_1 . Likewise, using an OA(81, 10, 9, 2) and $R_{10,1}^9$, a column-orthogonal LHD(81, 10) can be constructed, denoted by D_3 . It achieves a stratification on a 9×9 grid in any two dimensions, but has much less columns than that of D_1 . At last, for the design constructed by Ai, He and Liu [1], let us consider their Example 2.1. Suppose B is an OA(81, 10, 9, 2), and let

$$H = \begin{pmatrix} -8 & -6 & -4 & -2 & 0 & 2 & 4 & 6 & 8 \\ 4 & -2 & 6 & -4 & 0 & -8 & -6 & 2 & 8 \\ 4 & -2 & -8 & 8 & 0 & 2 & -6 & -4 & 6 \\ -6 & 8 & 2 & -4 & 0 & 4 & -2 & -8 & 6 \\ -2 & -4 & 4 & 6 & 0 & -6 & 8 & -8 & 2 \end{pmatrix}^T,$$

which is column-orthogonal and can be mapped into

$$Q = \begin{pmatrix} -2 & -2 & -2 & 0 & 0 & 0 & 2 & 2 & 2 \\ 2 & 0 & 2 & -2 & 0 & -2 & -2 & 0 & 2 \\ 2 & 0 & -2 & 2 & 0 & 0 & -2 & -2 & 2 \\ -2 & 2 & 0 & -2 & 0 & 2 & 0 & -2 & 2 \\ 0 & -2 & 2 & 2 & 0 & -2 & 2 & -2 & 0 \end{pmatrix}^T.$$

For all the $C_5^2 = 10$ pairs of columns of design Q , there are only three pairs of columns that can achieve combinatorial-orthogonality, i.e., the projection uniformity of Q is not so good. To obtain B^i , one replaces the 9 levels of $B \{-8, -6, \dots, 8\}$ with h_{1i}, \dots, h_{9i} , where h_{ji} is the (j, i) th element of H . Then $D_4 = (B^1 R_{10,1}^9, \dots, B^5 R_{10,1}^9)$ is a column-orthogonal LHD(81, 50). Repartition D_4 into 10 groups, where each group has five columns and the i th group consists of the i th columns of $B^j R_{10,1}^9$ with $j = 1, \dots, 5, i = 1, \dots, 10$. Then any two columns from different groups can achieve a stratification on a 9×9 grid, but there exist some pairs of columns from the same group that cannot achieve a stratification on a 3×3 grid. Comparing D_1, D_2, D_3 and D_4 , if we consider the number of columns and projection uniformity together, we see that D_1 is the most desirable one.

Example 4.4 Let A be the column-orthogonal MNOA(32; $(4^6)^5, (2^6)^5$) in Table 4. Rearrange the columns of A in the order of $\{1, 7, 13, 19, 25, 2, 8, 14, 20, 26, 3, 9, 15, 21, 27, 4, 10, 16, 22, 28, 5, 11, 17, 23, 29, 6, 12, 18, 24, 30\}$, we get a design $P = (P_1, \dots, P_6)$. Take $K = PR_{30,1}^4$, and rearrange its columns in the order of $\{1, 6, 11, 16, 21, 26, 2, 7, 12, 17, 22, 27, 3, 8, 13, 18, 23, 28, 4, 9, 14, 19, 24, 29, 5, 10, 15, 20, 25, 30\}$, then a column-orthogonal $D(32, 16^{30}; (4^6)^5, (2^6)^5)$ can be obtained, which is just the design constructed from A through Algorithm 4.1. The column-orthogonal $D(32, 16^{30}; (4^6)^5, (2^6)^5)$ is given in Table 6.

Space-filling designs with $N = \lambda n$ runs can be constructed by the method in this section, if (nearly) column-orthogonal MNOA($N; (s^u)^m, (p^u)^m$)’s can be constructed in Sect. 3, where the OA($n, m, s, 2$)’s should exist with $s = kp^\alpha, \lambda = 1$ or p and p must be a prime when $\alpha > 2$. Such orthogonal arrays can be found from Hedayat, Sloane and Stufken [6], e.g., saturated OA($s^2, s + 1, s, 2$)’s with s being a prime power, OA($2s^\beta, 2\frac{s^\beta-1}{s-1} - 1, s, 2$)’s with $\beta \geq 2$ being a positive integer and s being an odd prime power or $s = 2^b$ with b being a positive integer, OA($4s^\beta, 4\frac{s^\beta-1}{s-1} - 3, s, 2$)’s with s being an prime power and so on.

Sun and Tang [17] also constructed column-orthogonal $D(N, (s^2)^{um}; (s^u)^m, (p^u)^m)$ ’s by using OA($N, m, as, 2$)’s and OA($as, u, p, 2$)’s with a being a positive integer, requiring that u is a multiple of 4 or u and m are both even, and limiting $s = p^2$ which means that any two columns from different groups of the resulting design only achieve a stratification on a $p^2 \times p^2$ grid. They claimed that their designs have flexible parameters such as as and s are not required to be primes or prime powers. In fact, the proposed designs here have no such a requirement for s and p when $\alpha = 2$. For $\alpha > 2$, the proposed designs enjoy a much better space-filling property than those of Sun and Tang [17], i.e., any two columns from different groups of the newly constructed design can achieve a stratification on a $kp^\alpha \times kp^\alpha$ grid. Moreover, as u and m for their designs have some constraints, the numbers of columns of their designs are always less than or equal to those of ours.

Some resulting (nearly) column-orthogonal space-filling designs for $N < 1000$ are summarized in Table 7. In order to compare the resulting designs with those of Sun and Tang [17], we show the comparison results in the last column of Table 7. Here, the comparisons are made based on the following concerns. First, a good space-filling design should possess columns as many as possible, especially when being used as a screening

Table 6 continued

$D_2(32, 16^{30}; (4^6)^5, (2^6)^5)$

-5	-3	-5	-3	-1	13	15	9	15	9	-15	-9	-15	-9	-13	-1	-5	-3	-5	-3	5	3	5	3	1	-13	-15	-9	-15	-9
-3	5	-9	15	7	11	-13	-1	1	-13	-13	-1	7	11	-5	-3	9	-15	7	11	1	-13	-1	13	-15	-9	-1	13	3	-5
-7	-11	13	1	-9	15	-3	5	-13	-1	-11	7	11	-7	3	-5	-11	7	9	-15	3	-5	9	-15	-7	-11	13	1	-1	13
-1	13	1	-13	15	9	1	-13	-3	5	-9	15	-3	5	11	-7	7	11	-11	7	7	11	-13	-1	9	-15	3	-5	13	1
5	3	5	3	-7	-11	-15	-9	15	-5	-3	-5	-3	-9	15	15	9	11	-7	-15	-9	-15	-9	3	-5	-3	-7	-11	-7	-11
3	-5	9	-15	1	-13	13	1	-7	-11	-7	-11	13	1	-1	13	-3	5	-9	15	-11	7	11	-7	-13	-1	-11	7	11	-7
7	11	-13	-1	-15	-9	3	-5	11	-7	-1	13	1	-13	7	11	1	-13	-7	-11	-9	15	-3	5	-5	-3	7	11	-9	15
1	-13	-1	13	9	-15	-1	13	5	3	-3	5	-9	15	15	9	-13	-1	5	3	-13	-1	7	11	11	-7	9	-15	5	3
-9	-9	-15	-9	-5	-3	-5	-3	-1	13	5	3	5	3	-15	-9	-15	-9	-13	-1	-5	-3	-5	-3	7	11	15	9	9	-15
-9	15	-3	5	3	-5	7	11	-15	-9	7	11	-13	-1	-7	-11	3	-5	15	9	-1	13	1	-13	-9	15	1	-13	-5	-3
-13	-1	7	11	-13	-1	9	-15	3	-5	1	-13	-1	13	1	-13	-1	13	1	-13	-3	5	-9	15	-1	13	-13	-1	7	11
-11	7	11	-7	11	-7	-11	7	13	1	3	-5	9	-15	9	-15	13	1	-3	5	-7	-11	13	1	15	9	-3	5	-11	7
15	9	15	9	-3	5	5	3	7	11	15	9	15	9	-11	7	5	3	3	-5	15	9	15	9	5	3	5	3	1	-13
9	-15	3	-5	5	3	-7	-11	9	-15	13	1	-7	-11	-3	5	-9	15	-1	13	11	-7	-11	7	11	-7	-13	-1	-1	-13
13	1	-7	-11	-11	7	-9	15	-5	-3	11	-7	-11	7	5	3	11	-7	-15	-9	9	-15	3	-5	-3	5	-7	-11	15	9
11	-7	-11	7	13	1	11	-7	-11	7	9	-15	3	-5	13	1	-7	-11	13	1	13	1	-7	-11	13	1	-9	15	-3	5

Table 7 Some (nearly) column-orthogonal space-filling designs with $N < 1000$

$\lambda(k)$	B	D	Space-filling design	$C \alpha k m$
1	OA(16, 5, 4, 2)	T ₁	LHD(16, 10; (4 ²) ⁵ , (2 ²) ⁵)	> == >
2	OA(16, 5, 4, 2)	E ₃	$D(32, 16^{30}; (4^6)^5, (2^6)^5)$	> == <
1	OA(32, 9, 4, 2)	T ₁	$D(32, 16^{18}; (4^2)^9, (2^2)^9)$	> == >
2	OA(32, 9, 4, 2)	E ₃	$D(64, 16^{54}; (4^6)^9, (2^6)^9)$	> == >
1	OA(64, 21, 4, 2)	T ₁	$D(64, 16^{42}; (4^2)^{21}, (2^2)^{21})$	> == >
2	OA(64, 21, 4, 2)	E ₃	$D(128, 16^{126}; (4^6)^{21}, (2^6)^{21})$	> == >
1	OA(64, 9, 8, 2)	E ₁	LHD(64, 36; (8 ⁴) ⁹ , (2 ⁴) ⁹)	< > == >
1	OA(64, 9, 8, 2)	E ₁	LHD(64, 54; (8 ⁶) ⁹ , (2 ⁶) ⁹)*	> > == >
2	OA(64, 9, 8, 2)	E ₂	$D(128, 64^{108}; (8^{12})^9, (2^{12})^9)$ *	> > == <
1	OA(128, 17, 8, 2)	E ₁	$D(128, 64^{102}; (8^6)^{17}, (2^6)^{17})$ *	> > == >
1	OA(256, 17, 16, 2)	T ₁	LHD(256, 204; (16 ¹²) ¹⁷ , (2 ¹²) ¹⁷)	> (p is different)
1 ($k = 3$)	OA(144, 7, 12, 2)		LHD(144, 14; (12 ²) ⁷ , (2 ²) ⁷)	< == > >
1	OA(81, 10, 9, 2)	T ₁	LHD(81, 40; (9 ⁴) ¹⁰ , (3 ⁴) ¹⁰)	=====
3	OA(81, 10, 9, 2)	T ₅	$D(243, 81^{120}; (9^{12})_{10}, (3^{12})_{10})$	
1	OA(162, 19, 9, 2)	T ₁	$D(162, 81^{76}; (9^4)^{19}, (3^4)^{19})$	=====
1 ($k = 2$)	OA(648, 18, 18, 2)	E ₄	LHD(648, 72; (18 ⁴) ¹⁸ , (3 ⁴) ¹⁸)*	< == > =
1	OA(729, 91, 9, 2)	T ₁	$D(729, 81^{364}; (9^4)^{91}, (3^4)^{91})$	=====
1	OA(256, 17, 16, 2)	T ₁	LHD(256, 68; (16 ⁴) ¹⁷ , (4 ⁴) ¹⁷)	=====
1	OA(512, 33, 16, 2)	T ₁	$D(512, 256^{132}; (16^4)^{33}, (4^4)^{33})$	=====
1	OA(625, 26, 25, 2)	T ₁	LHD(625, 156; (25 ⁶) ²⁶ , (5 ⁶) ²⁶)	=====

Showing λ only in the first column means $k = 1$; B is the design B in Theorem 3.2; E_i means the design D in Theorem 3.2 is from Example i with $i = 1, 2, 3, 4$, and T_j means D is from Table with $j = 1$ and 5; all the designs are column-orthogonal except for the designs marked with “*” which are nearly column-orthogonal; the last column headed by “ $C \alpha k m$ ” show the results compared with those by Sun and Tang [17] on the following aspects: number of columns C , α , k , and m , where “>”, “=” or “<” means that the newly constructed design has a larger, the same, or smaller value of C , α , k or m than the corresponding design with the same number of runs by Sun and Tang [17]

design. Second, for a (nearly) column-orthogonal $D(N, (s^2)^{um}; (s^u)^m, (p^u)^m)$ with $N = \lambda n$, large k and α means that any one column and any two columns from different group can achieve a much better projection uniformity, i.e., each column has $(kp^\alpha)^2$ levels and the two columns can achieve a stratification on a $kp^\alpha \times kp^\alpha$ grid. Third, since the ratio π in (2.1) strictly increases with respect to m , we believe that a larger m means a better projection uniformity, specially for a fixed u . Thus, the comparisons are made in terms of the number of columns, α , k and m . The results show that most of the newly constructed designs have the same parameters as those of Sun and Tang [17], or even larger ones, for the same run sizes. And for some designs with the same run sizes, more constructions are available here, such as the designs with 64 runs in Table 7.

5 Concluding Remarks

The column-orthogonality and projection uniformity are two desirable properties for space-filling designs. Construction of designs with both properties is a challenging task. In this paper, we present some new methods for constructing designs with both (nearly) column-orthogonality and projection uniformity. For an ordinary MNOA($N; (s^u)^m, (p^u)^m$), any two columns from different groups can achieve combinatorial-orthogonality, then they must be column-orthogonal. But it did not guarantee that any two distinct columns from the same group can achieve column-orthogonality or even near column-orthogonality. Here we improve the column-orthogonality in each group. (Nearly) column-orthogonal MNOA($\lambda n; (s^u)^m, (p^u)^m$)'s were constructed under three situations. Furthermore, the constructed MNOAs are used to construct space-filling designs with more levels. The resulting $D(\lambda n, (s^2)^{um}; (s^u)^m, (p^u)^m)$'s not only preserve the multi-dimensional projection uniformity and column-orthogonality of the employed MNOAs, but also have a greater stratification in any one dimension. Comparisons with existing results show that the newly constructed designs enjoy much better projection uniformity and column-orthogonality, and can accommodate more columns, which can be regarded as fairly good space-filling designs for computer experiments.

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6 Appendix A Proofs of Theorems

6.1 Proof of Theorem 3.2

From Step 3, we know that A_j^w is a matrix obtained by replacing the levels of the j column of B , say b_{ij} , with the $(b_{ij} + s + 1)/2$ th row of D_w . That is, A_j^w contains all

the rows of D_w , and each row repeats n/s times. Then $A_j = (A_j^{1T}, A_j^{2T}, \dots, A_j^{\lambda T})^T$ has the same column-orthogonality and stratification as design D , which means that $\rho(A_j) = \rho(D)$ and A_j can achieve a stratification on a $p \times p$ grid in any two dimensions when design D can be mapped into an orthogonal array of p levels. For any two columns from A_i^w and A_j^w ($i \neq j$), respectively, we know they are obtained by permuting the levels of the i th and j th column of the design B which is an $OA(n, m, s, 2)$; then, they can achieve combinatorial-orthogonality based on s levels and p levels. So for any two columns from different groups A_i and A_j ($i \neq j$), they can also achieve combinatorial-orthogonality, and thus, they must be column-orthogonal. In conclusion, A is an MNOA($\lambda n; (s^u)^m, (p^u)^m$) with $\rho(A) = I_m \otimes \rho(D)$. \square

6.2 Proof of Theorem 3.4

The elements of $G_{i_1}(\pm p^0) + G_{i_2}(\pm p^1) + \dots + G_{i_\alpha}(\pm p^{\alpha-1})$ can be expressed as

$$g = g_1 \times (\pm 1) + g_2 \times (\pm p) + \dots + g_\alpha \times (\pm p^{\alpha-1}),$$

with $g_1, g_2, \dots, g_\alpha \in \{-p + 1 + 2(i - 1) : i = 1, 2, \dots, p\}$. Now let $\pm g_i = -p + 1 + b_i$, $i = 1, 2, \dots, \alpha - 1$, and $\pm g_\alpha = -p + 1 + 2(r - 1)$, where $b_1, b_2, \dots, b_{\alpha-1} \in \{0, 2, \dots, 2(p - 1)\}$, and $r = 1, \dots, p$, then

$$\begin{aligned} g &= (-p + 1) \sum_{i=1}^{\alpha} p^{i-1} + \sum_{i=1}^{\alpha-1} b_i p^{i-1} + 2(r - 1)p^{\alpha-1} \\ &= -(p^\alpha - 1) + \sum_{i=1}^{\alpha-1} b_i p^{i-1} + 2(r - 1)p^{\alpha-1} \\ &= -p^\alpha + 2(r - 1)p^{\alpha-1} + \sum_{i=1}^{\alpha-1} b_i p^{i-1} + 1. \end{aligned}$$

Since $\sum_{i=1}^{\alpha-1} b_i p^{i-1} \in \{0, 2, \dots, 2(p^{\alpha-1} - 1)\}$, it follows that

$$g \in [-p^\alpha + 2(r - 1)p^{\alpha-1} + 1, -p^\alpha + 2rp^{\alpha-1}),$$

i.e., g can be mapped to level $-p + 2r - 1 = \pm g_\alpha$. Through the above discussion, we know that when $G_{i_1}(\pm p^0) + G_{i_2}(\pm p^1) + \dots + G_{i_\alpha}(\pm p^{\alpha-1})$ is mapped to p levels, it becomes $\pm G_{i_\alpha}$. Since the t entries of $\pm p^{\alpha-1}$'s that in $R_{u,d}^p$ and $T_{u,\alpha,t}^p$ are both in different rows, then the conclusion is reached. \square

6.3 Proof of Theorem 3.6

Denote

$$G = (G_{ij}) = \left(2 \left(e_{ij} \oplus_b \frac{F + (p - 1)J_{p^\alpha \times f}}{2} \right) - (p - 1)J_{p^\alpha \times f} \right)_{pe},$$

where e_{ij} is the (i, j) th element of E . By Hedayat, Sloane and Stufken [6], we know that G is an $OA(p^{\alpha+1}, ef, p, 2)$, each G_{ij} is also an $OA(p^\alpha, f, p, 2)$ through permuting the levels of F , and the k th α consecutive columns of G_{ij} also compose a full factorial design $D(p^\alpha, p^\alpha)$, where $k = 1, \dots, v$. Then G is a resolvable $OA(p^{\alpha+1}, ef, p, 2)$ that can be resolvable into p parts and each part $G_i = (G_{i1}, \dots, G_{ie})$ is a $D(p^\alpha, p^{ef})$, in which the k th α consecutive columns compose a full factorial design, where $k = 1, \dots, ev$. From Lemma 3.3 and Theorem 3.4, results (ii) and (iii) can be derived. For $\alpha = 2$, we know that G_{ij}^f and $G_{i(j+1)}^1$ are obtained by permuting the levels of the f th and first columns of F , respectively, and then $(G_{ij}^f, G_{i(j+1)}^1)$ is an $OA(p^2, 2, p, 2)$, where G_{ij}^k is the k th column of G_{ij} . Thus the two consecutive columns of G_i in the order compose a full factorial design. Then result (i) can be similarly obtained. \square

6.4 Proof of Theorem 3.11

Let a be a level of L_i , then $a \in \{-\omega + 1, -\omega + 3, \dots, \omega - 1\}$. If L_i can be mapped into an $OA(\omega, u, p, 2)$, then ω must be a multiple of p^2 , denoted by $\omega = rp^2$, and all the levels $a \in [-\omega + 2(j - 1)\omega/p, -\omega + 2j\omega/p] = [-rp^2 + 2(j - 1)rp, -rp^2 + 2jrp]$ can be mapped to $-p + 2j - 1, j = 1, 2, \dots, p$. The elements of D can be expressed as

$$\begin{aligned} g &= k(-rp^2 + 2(j - 1)rp + b) + i \\ &= -krp^2 + 2(j - 1)krp + kb + i, \end{aligned}$$

with $j \in \{1, 2, \dots, p\}, b \in \{1, 3, \dots, 2rp - 1\}$ and $i \in \{-k + 1, -k + 3, \dots, k - 1\}$. Since $kb + i \in \{1, 3, \dots, 2krp - 1\}$, then when D is mapped to p levels, g becomes $-p + 2j - 1$. Through the above discussion, we know that D_i and L_i can become the same design when they are mapped to p levels. Then design D can be mapped into an $OA(kw, u, p, 2)$ when each design L_i can be mapped into an $OA(\omega, u, p, 2)$.

For the case of $\alpha = 2^d$, from (3.5), we know that

$$|\rho_{ij}(D)| = \theta |\rho_{ij}(H)| = \frac{k^2 - 1}{p^{2\alpha}k^2 - 1} |\rho_{ij}(H)| \leq \frac{k^2 - 1}{16k^2 - 1} |\rho_{ij}(H)| < 1/16 \text{ for } i \neq j,$$

so D is (nearly) column-orthogonal. Furthermore, when H is column-orthogonal, D is column-orthogonal with $\rho_{ij}(D) = \theta \rho_{ij}(H) = 0$ for $i \neq j$, and then $\rho(D) = I_u$.

For the case of $\alpha \neq 2^d$, we know that $\rho(L_i) = \rho(T_{u,\alpha,t})$. Then for $i \neq j$,

$$\begin{aligned} |\rho_{ij}(D)| &= |(1 - \theta)\rho_{ij}(T_{u,\alpha,t}) + \theta\rho_{ij}(H)| \\ &< |\rho_{ij}(T_{u,\alpha,t})| + \frac{k^2 - 1}{p^{2\alpha}k^2 - 1} |\rho_{ij}(H)| \\ &\leq |\rho_{ij}(T_{u,\alpha,t})| + \frac{k^2 - 1}{64k^2 - 1} |\rho_{ij}(H)| \\ &\leq |\rho_{ij}(T_{u,\alpha,t})| + \frac{1}{64}. \end{aligned}$$

\square

6.5 Proof of Theorem 4.2

As the absolute value of the (i, i) th element of $\begin{pmatrix} R_{a,1}^s \\ 0_{r \times a} \end{pmatrix}$ is s^2 , then according to the proof of Theorem 3.4, we know that K becomes $(P_1, \dots, P_{u-1}, P_{u1}, \dots, P_{u(m-r)})$ when it is mapped to s levels. That is to say, L becomes $(A_1, \dots, A_{m-1}, A_{m1}, \dots, A_{m(u-r)})$ when it is mapped to s levels. Then the projection uniformity is derived.

We now prove the column-orthogonality of K . Let $P = (P_1, \dots, P_u)$. It can be calculated that $\rho(K) = 3K^T K / (\lambda n(s^4 - 1))$, $\rho(P) = 3P^T P / (\lambda n(s^2 - 1))$ and $\rho(R_{a,1}^s) = (R_{a,1}^s)^T R_{a,1}^s / (s^2 + 1) = I_a$.

(1) If $\rho(D) = I_u$, then $\rho(A) = \rho(P) = I_{um}$. Let $R = \begin{pmatrix} R_{a,1}^s \\ 0_{r \times a} \end{pmatrix}$, then

$$\begin{aligned} \rho(K) &= \rho(P \cdot R) = \frac{3}{\lambda n(s^4 - 1)} (P \cdot R)^T (P \cdot R) \\ &= \frac{3}{\lambda n(s^4 - 1)} \cdot \frac{\lambda n(s^2 - 1)}{3} R^T R \\ &= \frac{1}{s^2 + 1} R^T R \\ &= I_a. \end{aligned}$$

So $\rho(L) = \rho(K) = I_a$.

(2) If m is even, then $R_{a,1}^s = I_u \otimes R_{m,1}^s$ where $a = um$. Besides, $\rho(P) = \rho(D) \otimes I_m$ when $\rho(A) = I_m \otimes \rho(D)$. Then

$$\begin{aligned} \rho(K) &= \rho(P \cdot R_{a,1}^s) = \frac{3}{\lambda n(s^4 - 1)} (P \cdot R_{a,1}^s)^T (P \cdot R_{a,1}^s) \\ &= \frac{3}{\lambda n(s^4 - 1)} (R_{a,1}^s)^T \cdot P^T P \cdot R_{a,1}^s \\ &= \frac{3}{\lambda n(s^4 - 1)} \cdot \frac{\lambda n(s^2 - 1)}{3} (I_u \otimes (R_{m,1}^s)^T) \cdot (\rho(D) \otimes I_m) \cdot (I_u \otimes R_{m,1}^s) \\ &= \frac{1}{s^2 + 1} \rho(D) \otimes ((R_{m,1}^s)^T R_{m,1}^s) \\ &= \rho(D) \otimes I_m. \end{aligned}$$

Then the correlation matrix of the constructed design is $\rho(L) = I_m \otimes \rho(D)$.

(3) When m is odd, we first prove the case of $r = 0$, i.e., m is odd and u is even. Set $a = um = 2b$ and let

$$\rho(D) \otimes I_m = \begin{pmatrix} V_{11} & \cdots & V_{1b} \\ \vdots & & \vdots \\ V_{b1} & \cdots & V_{bb} \end{pmatrix},$$

where V_{ij} is a 2×2 matrix. Besides, $R_{a,1}^s$ can be expressed as $R_{a,1}^s = I_b \otimes R_{2,1}^s$. Then

$$\rho(K) = \frac{1}{s^2 + 1} (R_{a,1}^s)^T \cdot (\rho(D) \otimes I_m) \cdot R_{a,1}^s = \frac{1}{s^2 + 1} ((R_{2,1}^s)^T V_{ij} R_{2,1}^s)_{um \times um},$$

where $(R_{2,1}^s)^T V_{ij} R_{2,1}^s$ is the (i, j) th submatrices of $(s^2 + 1)\rho(K)$ with order 2×2 . From the structure of $\rho(D) \otimes I_m$, we obtain that V_{ij} have the following three forms:

$$V_1 = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 & 0 \\ d_3 & 0 \end{pmatrix}, \quad \text{and} \quad V_3 = \begin{pmatrix} 0 & d_4 \\ 0 & 0 \end{pmatrix},$$

where d_i is the element of $\rho(D)$ with $|d_i| \leq 1$ and $i = 1, 2, 3, 4$, and $d_1 = d_2 = 1$ when V_1 is the (i, i) th submatrix of $\rho(D) \otimes I_m$ with $i = 1, 2, \dots, b$. Then

$$(R_{2,1}^s)^T V_1 R_{2,1}^s = \begin{pmatrix} d_1 s^2 + d_2 & -d_1 s + d_2 s \\ -d_1 s + d_2 s & d_1 + d_2 s^2 \end{pmatrix}, \quad (R_{2,1}^s)^T V_2 R_{2,1}^s = \begin{pmatrix} d_3 s & -d_3 \\ d_3 s^2 & -d_3 s \end{pmatrix},$$

$$\text{and} \quad (R_{2,1}^s)^T V_3 R_{2,1}^s = \begin{pmatrix} d_4 s & d_4 s^2 \\ -d_4 & -d_4 s \end{pmatrix}.$$

Denote $d = \max_{i < j} |\rho_{ij}(D)|$, then

$$\left| \frac{d_i}{1 + s^2} \right| \leq \left| \frac{d_i s}{1 + s^2} \right| \leq \frac{|d_i|s + |d_j|s}{1 + s^2} \leq \frac{ds^2}{1 + s^2} \leq \frac{ds^2 + d}{1 + s^2} = d, \quad \text{and}$$

$$\frac{1}{1 + s^2} (R_{2,1}^s)^T V_1 R_{2,1}^s = I_2$$

when $d_1 = d_2 = 1$. So we have $|\rho_{ij}(K)| \leq \rho_M(D)$, that is $|\rho_{ij}(L)| \leq \rho_M(D)$.

The case of $r = 1$ can be obtained similarly. So the column-orthogonality is derived. □

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