

Statistica Sinica Preprint No: SS-2020-0110

Title	Construction of strong group-orthogonal arrays
Manuscript ID	SS-2020-0110
URL	http://www.stat.sinica.edu.tw/statistica/
DOI	10.5705/ss.202020.0110
Complete List of Authors	Chunyan Wang, Jinyu Yang and Min-Qian Liu
Corresponding Author	Min-Qian Liu
E-mail	mqliu@nankai.edu.cn

CONSTRUCTION OF STRONG GROUP-ORTHOGONAL ARRAYS

Chunyan Wang, Jinyu Yang and Min-Qian Liu

Nankai University

Abstract: Space-filling designs with low-dimensional stratifications are desirable choices for computer experiments. In addition, column orthogonality is an important property of designs for such experiments, because it allows the estimates of the main effects in linear models to be uncorrelated with each other. However, few works have examined space-filling designs with both properties. This paper proposes a new class of designs called strong group-orthogonal arrays, the columns of which can be partitioned into groups, with the columns from different groups being column orthogonal and enjoying attractive low-dimensional stratifications. In addition, the overall arrays collapse to fully orthogonal arrays that accommodate large numbers of factors, making them particularly suitable for computer experiments. Methods for constructing this class of arrays based on both regular and nonregular designs are proposed. Difference schemes play a key role in the construction. Lastly, the proposed methods are easy to implement.

Key words and phrases: Column orthogonality, computer experiment, space-filling design, strong orthogonal array.

1. Introduction

Computer experiments are widely used in many fields, and space-filling designs are appropriate for such experiments (Fang, Li and Sudjianto (2006)). A space-filling design spreads its points in the design region uniformly, where the uniformity can

be evaluated using some distance or discrepancy criteria. For a design in a high-dimensional region, it may be more reasonable to consider its space-filling properties in low-dimensional projections. Numerous approaches have been proposed for constructing space-filling designs with good properties in low-dimensional projections using orthogonal arrays (OAs), or other arrays that can be collapsed into OAs, such as strong orthogonal arrays (SOAs) and mappable nearly orthogonal arrays (MNOAs). McKay, Beckman and Conover (1979) introduced Latin hypercube designs (LHDs), which are OAs of strength one. Owen (1992) and Tang (1993) considered randomized OAs and OA-based LHDs. Recently, He and Tang (2013, 2014) introduced SOAs and Mukerjee, Sun and Tang (2014) proposed MNOAs. Both arrays are better space-filling designs than those based on ordinary OAs. In addition to the space-filling property, column orthogonality is a desirable property for computer experiment designs, because it guarantees that the estimates of the main effects are uncorrelated with each other when polynomial modeling is considered.

Motivated by MNOAs and SOAs, we propose a new class of arrays called strong group-orthogonal arrays (SGOAs), the columns of which can be partitioned into groups, with the columns from different groups being column orthogonal and enjoying attractive low-dimensional space-filling properties. This class of arrays performs well in terms of both the space-filling property and column orthogonality, and can accommodate large numbers of factors. To see the benefits of such an array, consider the four arrays in Table 1; detailed definitions of these arrays are provided in Section 2. The column orthogonal SOA(8, 3, 4, 3-), denoted as OSOA(8, 3, 4, 3-), constructed in

Table 1: The OA(8,7,2,2), OSOA(8,3,4,3-), SOA(8,3,8,3), and SGOA(8,6,4,2).

OA(8,7,2,2)	OSOA(8,3,4,3-)	SOA(8,3,8,3)	SGOA(8,6,4,2)
0 0 0 0 0 0 0	3 3 3	0 0 0	0 0 0 0 0 0
0 0 1 0 1 1 1	0 3 0	2 3 6	0 0 3 3 3 3
0 1 0 1 0 1 1	3 0 0	3 6 2	3 3 0 0 3 3
0 1 1 1 1 0 0	0 0 3	1 5 4	3 3 3 3 0 0
1 0 0 1 1 0 1	1 1 1	6 2 3	1 2 1 2 1 2
1 0 1 1 0 1 0	2 1 2	4 1 5	1 2 2 1 2 1
1 1 0 0 1 1 0	1 2 2	5 4 1	2 1 1 2 2 1
1 1 1 0 0 0 1	2 2 1	7 7 7	2 1 2 1 1 2

Zhou and Tang (2019) can accommodate three factors, achieving stratifications (to be defined in Section 2) on 2×4 and 4×2 grids in any two dimensions, and a stratification on a $2 \times 2 \times 2$ grid in the three dimensions. This also holds for the SOA(8,3,8,3). The SOA(8,3,8,3) has eight levels and cannot guarantee column orthogonality. The SGOA(8,6,4,2) constructed in this paper can accommodate six factors, each of four levels. It guarantees stratifications on 2×4 and 4×2 grids and column orthogonality in 12 of the 15 two dimensions (80.00%), and stratifications on $2 \times 2 \times 2$ grids in 16 of the 20 three dimensions (80.00%). As summarized in Table 2, the SGOA(8,6,4,2) is nearly an OSOA of strength 3-, and can accommodate twice as many columns as the latter, making it a more economical choice.

Table 2: Properties of the OSOA(8,3,4,3-), SOA(8,3,8,3), and SGOA(8,6,4,2).

Design	Column orthogonality	Two-dimensional stratification	Three-dimensional stratification
OSOA(8,3,4,3-)	1	2×4 and 4×2	$2 \times 2 \times 2$
SOA(8,3,8,3)	No	2×4 and 4×2	$2 \times 2 \times 2$
SGOA(8,6,4,2)	80%	2×4 and 4×2 (80%)	$2 \times 2 \times 2$ (80%)

The SGOA(8,6,4,2) can be regarded as an intermediate between the OA(8,7,2,

2) and the OSOA(8, 3, 4, 3–). Correspondingly, an LHD based on the SGOA(8,6,4,2) can be regarded as an intermediate between those based on the OA(8, 7, 2, 2) and the SOA(8, 3, 8, 3), where the SOA(8, 3, 8, 3) is actually an LHD. According to Mukerjee, Sun and Tang (2014), an MNOA of eight runs with four levels is not available, implying that SGOAs have more flexible run sizes than MNOAs. These attractive properties make the SGOA(8, 6, 4, 2) a better choice for computer experiments.

The remainder of this paper is organized as follows. Section 2 introduces the definitions and notation used in this paper. In Section 3, we construct SGOAs of strength 2, and Section 4 constructs SGOAs of strength 3. Concluding remarks are provided in Section 5. All proofs and two large tables are deferred to the Supplementary Material.

2. Definitions and Notation

An $n \times m$ matrix is called an OA with strength t and s_1, \dots, s_m levels, denoted by $OA(n, m, s_1 \times \dots \times s_m, t)$, if all possible level combinations for any t columns occur with the same frequency. When all s_j are equal to s , the array is symmetric and denoted by $OA(n, m, s, t)$. Two vectors are called combinatorial-orthogonal if they form an OA of strength 2. The correlation between two vectors $a = (a_1, \dots, a_n)^T$ and $b = (b_1, \dots, b_n)^T$ is defined as

$$\rho(a, b) = \frac{\sum_{i=1}^n (a_i - \bar{a})(b_i - \bar{b})}{\left[\sum_{i=1}^n (a_i - \bar{a})^2 \sum_{i=1}^n (b_i - \bar{b})^2 \right]^{1/2}},$$

where $\bar{a} = \sum_{i=1}^n a_i/n$ and $\bar{b} = \sum_{i=1}^n b_i/n$. Two vectors are called column orthogonal if the correlation between them is zero. The correlation matrix of a design D is denoted by $\rho(D) = (\rho(d_i, d_j))_{m \times m}$, where d_i and d_j are the i th and j th columns, respectively,

of D , for $1 \leq i, j \leq m$. A design is called column orthogonal if any two of its columns are column orthogonal.

For an array with n runs and m factors, we say it achieves a stratification on an $s_1 \times \cdots \times s_t$ grid in some t ($t \geq 2$) dimensions if its corresponding t columns can be collapsed into an $OA(n, t, s_1 \times \cdots \times s_t, t)$.

A design is called a regular design if any two of its factorial effects are either combinatorial-orthogonal to each other or are fully aliased.

An LHD of n runs and m factors is an $n \times m$ matrix in which each column is a permutation of $0, 1, \dots, n - 1$. An LHD based on a q -level design of n runs, with n being a multiple of q , can be obtained by replacing the n/q entries for level j of each factor by any permutation of $jn/q, jn/q + 1, \dots, (j + 1)n/q - 1$, for $j = 0, 1, \dots, q - 1$.

Let $GF(s)$ denote the Galois field with order s . An $r \times c$ matrix with entries from $GF(s)$ is called a difference scheme based on $GF(s)$, denoted by $D(r, c, s)$, if it satisfies that for any i and j with $1 \leq i \neq j \leq c$, the vector difference of the i th and j th columns contains every element of $GF(s)$ equally often.

For two matrices $A = (a_{ij})_{m \times n}$ and $B = (b_{ij})_{u \times v}$ with entries from $GF(s)$, their Kronecker sum and Kronecker product are defined as

$$A \oplus B = \begin{pmatrix} a_{11} \dot{+} B & \cdots & a_{1n} \dot{+} B \\ \vdots & & \vdots \\ a_{m1} \dot{+} B & \cdots & a_{mn} \dot{+} B \end{pmatrix} \text{ and } A \otimes B = \begin{pmatrix} a_{11} \dot{\times} B & \cdots & a_{1n} \dot{\times} B \\ \vdots & & \vdots \\ a_{m1} \dot{\times} B & \cdots & a_{mn} \dot{\times} B \end{pmatrix}, \quad (2.1)$$

respectively, where $\dot{+}$ and $\dot{\times}$ are the addition and multiplication, respectively, defined on $GF(s)$.

The operator $*$ is a right circular shift of the columns of a design, which means

that for a design $D = (d_1, \dots, d_s)$, $D^* = (d_s, d_1, \dots, d_{s-1})$.

An MNOA, denoted by $\text{MNOA}\{n; (s^\mu)^\phi, (p^\mu)^\phi\}$, is an $n \times \mu\phi$ array in which the $\mu\phi$ columns can be partitioned into ϕ disjoint groups of μ columns, each with the following properties:

- (i) every column is populated by s levels from $GF(s)$;
- (ii) any two columns from different groups form an $\text{OA}(n, 2, s, 2)$;
- (iii) the whole design can be collapsed into an $\text{OA}(n, \mu\phi, p, 2)$, where the s levels of each column are collapsed into p levels by $\lfloor x/(s/p) \rfloor$, for $x = 0, 1, \dots, s - 1$, with s/p being a positive integer, and $\lfloor z \rfloor$ representing the largest integer not exceeding z .

In such an array, each column is combinatorial-orthogonal to at least a proportion $\tilde{\pi} = (\phi - 1)\mu/(\phi\mu - 1)$ of the other columns.

An $n \times m$ matrix with entries from $\{0, 1, \dots, s^t - 1\}$ is called an SOA of strength t , denoted by $\text{SOA}(n, m, s^t, t)$, if any $n \times f$ submatrix, for $1 \leq f \leq t$, can be collapsed into an $\text{OA}(n, f, s^{\mu_1} \times \dots \times s^{\mu_f}, f)$ for any positive integers μ_1, \dots, μ_f , with $\mu_1 + \dots + \mu_f = t$, where the s^t levels of a factor are collapsed into s^{μ_j} levels by $\lfloor x/s^{t-\mu_j} \rfloor$, for $x = 0, 1, \dots, s^t - 1, 1 \leq j \leq f$. Furthermore, an $n \times m$ matrix with entries from $\{0, 1, \dots, s^2 - 1\}$ is called an SOA of strength $2+$, denoted by $\text{SOA}(n, m, s^2, 2+)$, if any submatrix of two columns can be collapsed into an $\text{OA}(n, 2, s^2 \times s, 2)$ and an $\text{OA}(n, 2, s \times s^2, 2)$. An $n \times m$ matrix with entries from $\{0, 1, \dots, s^2 - 1\}$ is called an SOA of strength $3-$, denoted by $\text{SOA}(n, m, s^2, 3-)$, if any submatrix of two columns

can be collapsed into an $OA(n, 2, s^2 \times s, 2)$ and an $OA(n, 2, s \times s^2, 2)$, and any submatrix of three columns can be collapsed into an $OA(n, 3, s, 3)$.

For an $SOA(n, m, s^t, t)$, if it is column orthogonal, we call it a column orthogonal SOA of strength t , denoted by $OSOA(n, m, s^t, t)$. Similarly, we have $OSOA(n, m, s^2, 2+)$ and $OSOA(n, m, s^2, 3-)$.

Table 3: An $SGOA(27, 12, 9, 2)$.

Pre-collapsing				Post-collapsing			
T_1	T_2	T_3	T_4	A_1	A_2	A_3	A_4
0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
0 0 0	4 4 4	4 4 4	8 8 8	0 0 0	1 1 1	1 1 1	2 2 2
0 0 0	8 8 8	8 8 8	4 4 4	0 0 0	2 2 2	2 2 2	1 1 1
4 4 4	0 0 0	4 4 4	4 4 4	1 1 1	0 0 0	1 1 1	1 1 1
4 4 4	4 4 4	8 8 8	0 0 0	1 1 1	1 1 1	2 2 2	0 0 0
4 4 4	8 8 8	0 0 0	8 8 8	1 1 1	2 2 2	0 0 0	2 2 2
8 8 8	0 0 0	8 8 8	8 8 8	2 2 2	0 0 0	2 2 2	2 2 2
8 8 8	4 4 4	0 0 0	4 4 4	2 2 2	1 1 1	0 0 0	1 1 1
8 8 8	8 8 8	4 4 4	0 0 0	2 2 2	2 2 2	1 1 1	0 0 0
2 3 7	2 3 7	2 3 7	2 3 7	0 1 2	0 1 2	0 1 2	0 1 2
2 3 7	3 7 2	3 7 2	7 2 3	0 1 2	1 2 0	1 2 0	2 0 1
2 3 7	7 2 3	7 2 3	3 7 2	0 1 2	2 0 1	2 0 1	1 2 0
3 7 2	2 3 7	3 7 2	3 7 2	1 2 0	0 1 2	1 2 0	1 2 0
3 7 2	3 7 2	7 2 3	2 3 7	1 2 0	1 2 0	2 0 1	0 1 2
3 7 2	7 2 3	2 3 7	7 2 3	1 2 0	2 0 1	0 1 2	2 0 1
7 2 3	2 3 7	7 2 3	7 2 3	2 0 1	0 1 2	2 0 1	2 0 1
7 2 3	3 7 2	2 3 7	3 7 2	2 0 1	1 2 0	0 1 2	1 2 0
7 2 3	7 2 3	3 7 2	2 3 7	2 0 1	2 0 1	1 2 0	0 1 2
1 6 5	1 6 5	1 6 5	1 6 5	0 2 1	0 2 1	0 2 1	0 2 1
1 6 5	5 1 6	5 1 6	6 5 1	0 2 1	1 0 2	1 0 2	2 1 0
1 6 5	6 5 1	6 5 1	5 1 6	0 2 1	2 1 0	2 1 0	1 0 2
5 1 6	1 6 5	5 1 6	5 1 6	1 0 2	0 2 1	1 0 2	1 0 2
5 1 6	5 1 6	6 5 1	1 6 5	1 0 2	1 0 2	2 1 0	0 2 1
5 1 6	6 5 1	1 6 5	6 5 1	1 0 2	2 1 0	0 2 1	2 1 0
6 5 1	1 6 5	6 5 1	6 5 1	2 1 0	0 2 1	2 1 0	2 1 0
6 5 1	5 1 6	1 6 5	5 1 6	2 1 0	1 0 2	0 2 1	1 0 2
6 5 1	6 5 1	5 1 6	1 6 5	2 1 0	2 1 0	1 0 2	0 2 1

Before giving the definition of the new class of SGOAs, first consider the array in

the left part of Table 3. It has twelve columns, each of which is populated by nine levels. If we partition these columns into four disjoint groups of three columns each in column order, the array has the following interesting properties:

- (i) any two distinct columns can be collapsed into an $OA(27, 2, 3, 2)$;
- (ii) any two columns from different groups are column orthogonal, and they can be collapsed into an $OA(27, 2, 3 \times 9, 2)$ and an $OA(27, 2, 9 \times 3, 2)$ using different collapsing methods;
- (iii) any three distinct columns from two different groups can be collapsed into an $OA(27, 3, 3, 3)$.

Definition 1. An SGOA of strength t , denoted by $SGOA(n, gc, s^t, t)$, is an $n \times gc$ matrix with entries from $\{0, 1, \dots, s^t - 1\}$ that can be partitioned into g disjoint groups of c columns, each with the following properties:

- (i) any two distinct columns can be collapsed into an $OA(n, 2, s \times s^{t-1}, 2)$ and an $OA(n, 2, s^{t-1} \times s, 2)$ using different collapsing methods;
- (ii) any two columns from different groups are column orthogonal, and they can be collapsed into an $OA(n, 2, s \times s^t, 2)$ and an $OA(n, 2, s^t \times s, 2)$ using different collapsing methods;
- (iii) any three distinct columns from two different groups can be collapsed into an $OA(n, 3, s, 3)$.

The array in Table 3 is an $SGOA(27, 12, 9, 2)$. Because an $SGOA(n, gc, s^t, t)$ with $t \geq 2$ can be collapsed into an $OA(n, gc, s, 2)$, we must have $n = \lambda s^2$, for some integer

λ . We call λ the index of an SGOA in the same way as that of an OA. Note that the strength t of an SGOA is an index that measures the space-filling property in two dimensions, where a larger t indicates that an SGOA is more space-filling in two dimensions. For an SGOA($n, gc, s^2, 2$), if $c = 1$ (i.e., each group has only one column), it becomes an OSOA($n, g, s^2, 2+$). Thus, an SGOA of strength 2 can be seen as a generalization of an OSOA of strength 2+. Furthermore, in an SGOA(n, gc, s^t, t), each column is column orthogonal to $gc - c$ columns among all other $gc - 1$ columns, and the corresponding pairs of columns can be collapsed into an OA($n, 2, s \times s^t, 2$) and an OA($n, 2, s^t \times s, 2$). For an SGOA(n, gc, s^t, t) with $t \geq 2$, we use π to denote the proportion of two-tuples that achieve stratifications on $s \times s^t$ and $s^t \times s$ grids and column orthogonality simultaneously; here,

$$\pi = (gc - c)/(gc - 1).$$

Similarly, we use δ to denote the proportion of three-tuples that achieve stratifications on $s \times s \times s$ grids. From the definition, any three distinct columns from two different groups can be collapsed into an OA($n, 3, s, 3$). Thus, the δ -value of any SGOA(n, gc, s^t, t) is at least δ_0 , with

$$\delta_0 = 3c(c - 1)(g - 1)/\{(gc - 1)(gc - 2)\}.$$

In fact, after some calculations, we find that the δ -value of an SGOA is often larger than δ_0 , and under some conditions, we obtain SGOAs with much larger δ -values.

3. Construction of SGOAs of Strength 2

In this section, we provide a general construction method for SGOAs of strength

2. Because the general method may not be easy to understand without examples, we first present two examples to illustrate the main idea.

Table 4: The OA(9, 4, 3, 2) in Example 1.

c_1	c_2	c_3	c_4
0	0	0	0
0	1	1	2
0	2	2	1
1	0	1	1
1	1	2	0
1	2	0	2
2	0	2	2
2	1	0	1
2	2	1	0

Example 1. Given an OA(9, 4, 3, 2) with entries from $GF(3)$, denoted by $C = (c_1, c_2, c_3, c_4)$, as shown in Table 4, we obtain an SGOA(27, 12, 9, 2) as follows. For $i = 1, 2, 3, 4$, let

$$A_i = \begin{pmatrix} c_i & c_i & c_i \\ c_i & c_i + 1 & c_i + 2 \\ c_i & c_i + 2 & c_i + 1 \end{pmatrix} \text{ and } B_i = \begin{pmatrix} c_i & c_i & c_i \\ c_i + 2 & c_i & c_i + 1 \\ c_i + 1 & c_i & c_i + 2 \end{pmatrix},$$

where $+$ is the addition defined on $GF(3)$. Treat all entries as numbers, and define $T_i = 3A_i + B_i$, for $i = 1, 2, 3, 4$. Then, we obtain an SGOA(27, 12, 9, 2) by taking $\tilde{T} = (T_1, T_2, T_3, T_4)$, which is shown in the left part of Table 3 and has the properties mentioned before Definition 1. It is easy to check that after level-collapsing by $\lfloor x/3 \rfloor$, \tilde{T} becomes $A = (A_1, A_2, A_3, A_4)$, which is an OA(27, 12, 3, 2), as shown in the right part of Table 3. For the resulting \tilde{T} , we have the proportion $\pi = 81.82\%$. Furthermore, by checking all three-tuples, we find that \tilde{T} achieves stratifications on $3 \times 3 \times 3$ grids in 180 of the 220 three dimensions, that is, $\delta = 81.82\%$, which is much larger than $\delta_0 = 49.09\%$.

Table 5: The OA(16, 5, 4, 2) in Example 2.

c_1	c_2	c_3	c_4	c_5
0	0	0	0	0
0	1	1	1	1
0	2	2	2	2
0	3	3	3	3
1	0	1	2	3
1	1	0	3	2
1	2	3	0	1
1	3	2	1	0
2	0	2	3	1
2	1	3	2	0
2	2	0	1	3
2	3	1	0	2
3	0	3	1	2
3	1	2	0	3
3	2	1	3	0
3	3	0	2	1

Example 2. We now construct an SGOA(64, 20, 16, 2). Let $C = (c_1, \dots, c_5)$ be an OA(16, 5, 4, 2) with entries from $GF(4)$, as shown in Table 5. For $i = 1, \dots, 5$, define

$$A_i = \begin{pmatrix} c_i & c_i & c_i & c_i \\ c_i & c_i + 1 & c_i + 2 & c_i + 3 \\ c_i & c_i + 2 & c_i + 3 & c_i + 1 \\ c_i & c_i + 3 & c_i + 1 & c_i + 2 \end{pmatrix} \text{ and } B_i = \begin{pmatrix} c_i & c_i & c_i & c_i \\ c_i + 3 & c_i & c_i + 1 & c_i + 2 \\ c_i + 1 & c_i & c_i + 2 & c_i + 3 \\ c_i + 2 & c_i & c_i + 3 & c_i + 1 \end{pmatrix},$$

where $+$ is the addition defined on $GF(4)$. Treat all entries as numbers, and create $T_i = 4A_i + B_i$, for $i = 1, \dots, 5$. We obtain an SGOA(64, 20, 16, 2) by taking $\tilde{T} = (T_1, T_2, T_3, T_4, T_5)$, which is shown in the left part of Table S.1 in the Supplementary Material. It is easy to check that after level-collapsing by $\lfloor x/4 \rfloor$, \tilde{T} becomes $A = (A_1, A_2, A_3, A_4, A_5)$, which is an OA(64, 20, 4, 2), as shown in the right part of Table S.1 in the Supplementary Material. For \tilde{T} , we can check that any two columns from different groups are column orthogonal and can be collapsed into an OA(64, 2, 4×16 , 2)

and an $\text{OA}(64, 2, 16 \times 4, 2)$, where the proportion π is 84.21%. We can also check that any three distinct columns from two different groups of \tilde{T} can be collapsed into an $\text{OA}(64, 3, 4, 3)$ with $\delta_0 = 480/1140 = 42.11\%$. Furthermore, by checking all three-tuples, we find that \tilde{T} achieves stratifications on $4 \times 4 \times 4$ grids in 960 of the 1140 three dimensions; that is, $\delta = 84.21\%$.

Next, we present the construction of SGOAs of strength 2 and investigate their properties. The construction method is given in the following algorithm.

Algorithm 1.

Step 1. For a prime power s , let $C = (c_1, \dots, c_g)$ be an $\text{OA}(n_0, g, s, 2)$ with entries from $GF(s)$ and D be a difference scheme $D(s, s, s)$. For $i = 1, \dots, g$, create

$$A_i = D \oplus c_i, \quad B_i = D^* \oplus c_i,$$

where \oplus is defined in (2.1), and D^* is the right circular shift design of D , as given in Section 2.

Step 2. Treat all entries as numbers, and define

$$T_i = sA_i + B_i, \quad \text{for } i = 1, \dots, g.$$

Step 3. Combine T_i by column juxtaposition, and get $\tilde{T} = (T_1, \dots, T_g)$.

For the resulting design, we have the following theorem.

Theorem 1. *The obtained \tilde{T} in Algorithm 1 is an $\text{SGOA}(sn_0, gs, s^2, 2)$; that is, \tilde{T} has the properties mentioned in Definition 1 with $n = sn_0, c = s$, and $t = 2$.*

Remark 1. In Algorithm 1, if D is a difference scheme $D(s, h, s)$, where $h \leq s$, then \tilde{T} is an $\text{SGOA}(sn_0, gh, s^2, 2)$. In particular, if D is $(0, 1, \dots, s-1)^T$, a difference scheme $D(s, 1, s)$, then \tilde{T} is an $\text{OSOA}(sn_0, g, s^2, 2+)$.

From Remark 1, there is a close relationship between the SGOA of strength 2 and the OSOA of strength 2+. Actually, if we take one column from each group of an $\text{SGOA}(n, gc, s^2, 2)$ and put these columns together, we obtain an $\text{OSOA}(n, g, s^2, 2+)$. In this sense, SGOAs of strength 2 can be regarded as a generalized version of OSOAs of strength 2+, where the proportion π measures the degree of proximity in terms of both column orthogonality and the two-dimensional space-filling property.

Remark 2. Let

$$\zeta = (0, \dots, 0, 1, \dots, 1, \dots, s-1, \dots, s-1)^T,$$

where each of $0, 1, \dots, s-1$ repeats n_0 times. In Algorithm 1, if C is saturated, then after collapsing all factors into s levels, \tilde{T} augmented by ζ is a saturated OA with s levels as well. This implies that the number of columns of the resulting SGOA is one less than that of the saturated OA with s levels and the same number of runs.

From Theorem 1, we know that \tilde{T} achieves stratifications on $s \times s^2$ and $s^2 \times s$ grids in any two columns from different groups, and a stratification on an $s \times s \times s$ grid in any three distinct columns from two different groups. In general, for an SGOA of strength 2, the δ -value is usually smaller than the π -value. When taking C to be some specified OAs, we get some SGOAs with large δ -values, which means that the resulting designs enjoy a better space-filling property in three dimensions. We are ready to present the next theorem.

Theorem 2. *If C in Algorithm 1 is saturated and regular, then the resulting \tilde{T} achieves stratifications on $s \times s \times s$ grids with a proportion π ; that is, $\delta = \pi$.*

From Theorem 2, many SGOAs enjoy the attractive space-filling properties in both two and three dimensions. The OAs and difference schemes needed in Algorithm 1 are available in Hedayat, Sloane and Stufken (1999) and the library of OAs maintained by Dr. N.J.A. Sloane (<http://neilsloane.com/oadir/index.html>). Table 6 summarizes some generated SGOAs of strength 2. Here, the symbol \ddagger means that the number of columns of the resulting SGOA is one less than that of the saturated OA with s levels and the same number of runs. The symbol \dagger means that if C is a saturated regular design, then the resulting SGOA can achieve stratifications on $s \times s \times s$ grids with a proportion π . As shown in Table 6, most of the values of π are very close to one, implying that the resulting designs enjoy attractive space-filling properties and column orthogonality.

Table 7 compares SGOAs, the MNOAs in Mukerjee, Sun and Tang (2014), and the SOAs in He, Cheng and Tang (2018), Liu and Liu (2015), and Zhou and Tang (2019).

As discussed, SGOAs of strength 2 can be regarded as a generalized version of OSOAs of strength 2+, where the proportion π measures the degree of proximity in terms of both column orthogonality and the two-dimensional space-filling property. From Table 7, we can see that the values of π are very close to one, which means that these SGOAs of strength 2 have almost the same desirable column orthogonality and two-dimensional space-filling properties as those of the OSOAs of strength 2+. In addition, they can accommodate s times as many columns as the latter can, and they

Table 6: Some SGOAs of strength 2.

$C: OA(n_0, g, s, 2)$	$\tilde{T}: SGOA(sn_0, gs, s^2, 2)$	$\pi(\%)$
OA(4, 3, 2, 2)	SGOA(8, 6, 4, 2) $\#\#$	80.00
OA(8, 7, 2, 2)	SGOA(16, 14, 4, 2) $\#\#$	92.31
OA(12, 11, 2, 2)	SGOA(24, 22, 4, 2) $\#$	95.24
OA(16, 15, 2, 2)	SGOA(32, 30, 4, 2) $\#\#$	96.55
OA(20, 19, 2, 2)	SGOA(40, 38, 4, 2) $\#$	97.30
OA(24, 23, 2, 2)	SGOA(48, 46, 4, 2) $\#$	97.78
OA(28, 27, 2, 2)	SGOA(56, 54, 4, 2) $\#$	98.11
OA(32, 31, 2, 2)	SGOA(64, 62, 4, 2) $\#\#$	98.36
OA(36, 35, 2, 2)	SGOA(72, 70, 4, 2) $\#$	98.55
OA(40, 39, 2, 2)	SGOA(80, 78, 4, 2) $\#$	98.70
OA(44, 43, 2, 2)	SGOA(88, 86, 4, 2) $\#$	98.82
OA(48, 47, 2, 2)	SGOA(96, 94, 4, 2) $\#$	98.92
OA(52, 51, 2, 2)	SGOA(104, 102, 4, 2) $\#\#$	99.01
OA(56, 55, 2, 2)	SGOA(112, 110, 4, 2) $\#\#$	99.08
OA(60, 59, 2, 2)	SGOA(120, 118, 4, 2) $\#\#$	99.15
OA(64, 63, 2, 2)	SGOA(128, 126, 4, 2) $\#\#$	99.20
OA(68, 67, 2, 2)	SGOA(136, 132, 4, 2) $\#\#$	99.25
OA(72, 71, 2, 2)	SGOA(144, 142, 4, 2) $\#\#$	99.29
OA(76, 75, 2, 2)	SGOA(152, 150, 4, 2) $\#\#$	99.33
OA(80, 79, 2, 2)	SGOA(160, 158, 4, 2) $\#\#$	99.36
OA(84, 83, 2, 2)	SGOA(168, 166, 4, 2) $\#\#$	99.39
OA(88, 87, 2, 2)	SGOA(176, 174, 4, 2) $\#\#$	99.42
OA(92, 91, 2, 2)	SGOA(184, 182, 4, 2) $\#\#$	99.45
OA(96, 95, 2, 2)	SGOA(192, 190, 4, 2) $\#\#$	99.47
OA(100, 99, 2, 2)	SGOA(200, 198, 4, 2) $\#\#$	99.49
OA(9, 4, 3, 2)	SGOA(27, 12, 9, 2) $\#\#$	81.82
OA(18, 7, 3, 2)	SGOA(54, 21, 9, 2)	90.00
OA(27, 13, 3, 2)	SGOA(81, 39, 9, 2) $\#\#$	94.74
OA(54, 25, 3, 2)	SGOA(162, 75, 9, 2)	97.30
OA(81, 40, 3, 2)	SGOA(243, 120, 9, 2) $\#\#$	98.32
OA(16, 5, 4, 2)	SGOA(64, 20, 16, 2) $\#\#$	84.21
OA(32, 9, 4, 2)	SGOA(128, 36, 16, 2)	91.43
OA(64, 21, 4, 2)	SGOA(256, 84, 16, 2) $\#\#$	96.39
OA(25, 6, 5, 2)	SGOA(125, 30, 25, 2) $\#\#$	86.21
OA(50, 11, 5, 2)	SGOA(250, 55, 25, 2)	92.59

perform better in three dimensions. OSOAs of strength 2 are better than SGOAs of strength 2 in terms of column orthogonality, and can accommodate more (or equally many) factors; SGOAs of strength 2 enjoy better two- and three-dimensional space-filling properties. Compared with the MNOAs constructed in Mukerjee, Sun and Tang (2014), the resulting SGOAs have a better three-dimensional space-filling property when the MNOAs are available. Furthermore, SGOAs are particularly useful when the

Table 7: Comparisons between SGOAs of strength 2, MNOAs, SOAs, and OSOAs.

s	n	SGOA($n, gs, s^2, 2$)		MNOA ¹		SOA(2+) ²	OSOA(2) ³	OSOA(p) ⁴	
		$\pi(\%)$	gs	$\bar{\pi}(\%)$	$\mu\phi$	m	m	m	p
2	8	80.00	6	—	—	—	—	3	3—
2	24,40,48 56,72,80 88,96,104 112,120 136,144,152 160,168,176 184,192,200	$\frac{n-4}{n-3}$	$n-2$	—	—	—	—	$n/2-1$	3—
2	16	92.31	14	85.71	15	10	14	7	3—
2	32	96.55	30	82.76	30	22	30	15	3—
2	64	98.36	62	96.77	63	50	62	31	3—
2	128	99.20	126	98.36	123	106	126	63	3—
3	27	81.82	12	—	—	6	12	4	2+
3	54	90.00	21	—	—	—	24	7	2+
3	81	94.74	39	92.31	40	25	40	13	2+
3	162	97.30	75	91.30	70	—	78	25	2+
3	243	98.32	120	90.76	120	90	120	40	2+
4	64	84.21	20	—	—	8	20	5	2+
4	128	91.43	36	—	—	—	40	9	2+
4	256	96.39	84	95.24	85	45	84	21	2+
5	125	96.39	30	—	—	10	30	6	2+
5	250	92.59	55	—	—	—	60	11	2+

¹MNOA $\{n, \mu m, ((s^2)^\mu)^\phi, (s^\mu)^\phi\}$ in Mukerjee, Sun and Tang (2014); ²SOA($n, m, s^2, 2+$) in He, Cheng and Tang (2018); ³OSOA($n, m, s^2, 2$) in Liu and Liu (2015); ⁴OSOA(n, m, s^2, p) in Zhou and Tang (2019); Symbol — indicates that the corresponding array is not available.

run size n is a multiple of s^3 , but not of s^4 , when the MNOAs are not available. That is, SGOAs can fill the gap between the run sizes of the available MNOAs. For example, we can construct SGOAs of 27 and 54 runs, whereas such MNOAs are not available. These desirable properties ensure that SGOAs are competitive designs for computer experiments. Figure 1 summaries the sizes of the designs listed in Table 7 for $s = 2$, where each point represents the design of the corresponding type with n runs and m

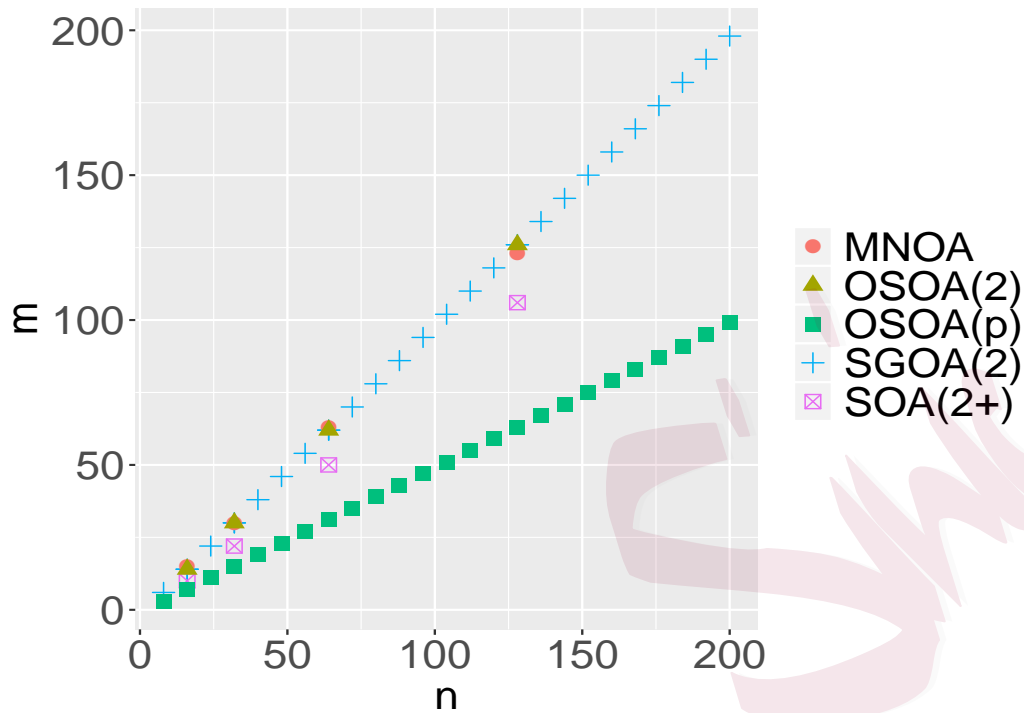


Figure 1: Comparison of SGOAs of strength 2 with some related designs for $s = 2$.

factors. We can see that SGOAs have flexible run sizes and can accommodate large numbers of factors.

4. Construction of SGOAs of Strength 3

In this section, we consider SGOAs of strength 3, in the sense that the factors have s^3 levels and their two-dimensional space-filling properties are better than those of SGOAs of strength 2. From Definition 1, we know that an SGOA of strength 3, denoted by $\text{SGOA}(n, gc, s^3, 3)$, is an $n \times gc$ matrix with entries from $\{0, 1, \dots, s^3 - 1\}$ that can be partitioned into g disjoint groups of c columns, each with the following properties:

- (i) any two distinct columns can be collapsed into an $\text{OA}(n, 2, s \times s^2, 2)$ and an

$OA(n, 2, s^2 \times s, 2)$ using different collapsing methods;

(ii) any two columns from different groups are column orthogonal, and can be collapsed into an $OA(n, 2, s \times s^3, 2)$ and an $OA(n, 2, s^3 \times s, 2)$ using different collapsing methods;

(iii) any three distinct columns from two different groups can be collapsed into an $OA(n, 3, s, 3)$.

Example 3. In Table S.2 in the Supplementary Material, the design $\bar{T} = (T_1, T_2, T_3, T_4)$ in the left part is an SGOA(81, 12, 27, 3), where each of the 12 columns is populated by 27 levels. It is easy to check that any two distinct columns can be collapsed into an $OA(81, 2, 3 \times 9, 2)$ and an $OA(81, 2, 9 \times 3, 2)$. Any two columns from different groups are column orthogonal, and they can be collapsed into an $OA(81, 2, 3 \times 27, 2)$ and an $OA(81, 2, 27 \times 3, 2)$; thus, we have $\pi = 81.82\%$. In addition, the maximum correlation coefficient between any two distinct columns from one group is 0.033, implying that \bar{T} is nearly column orthogonal. Collapsing each factor into three levels, we get an OA, which is displayed in the right part of Table S.2 in the Supplementary Material. We can see that any three distinct columns from two different groups form an $OA(81, 3, 3, 3)$. Thus, \bar{T} achieves stratifications on $3 \times 3 \times 3$ grids in at least 108 of the 220 three dimensions; that is, $\delta_0 = 49.09\%$. In fact, by checking all three-tuples, we find that \bar{T} achieves stratifications on $3 \times 3 \times 3$ grids in 207 of the 220 three dimensions; that is, $\delta = 94.09\%$. Thus, the design enjoys attractive space-filling properties in both two and three dimensions, as well as near column orthogonality.

Now, we introduce the method for constructing SGOAs of strength 3 in the following algorithm, and then discuss the properties of the resulting designs.

Algorithm 2.

Step 1. For a prime power s , let $C = (c_1, \dots, c_g)$ be an $OA(n_0, g, s, 2)$ with entries from $GF(s)$ and D be a difference scheme $D(s, s, s)$. For $i = 1, \dots, g$, create

$$E_i = (D^T, D_1^T, \dots, D_{s-1}^T)^T \oplus c_i, F_i = (1_s \otimes D^*) \oplus c_i, \text{ and } G_i = (1_s \otimes D^{**}) \oplus c_i,$$

where $D_k = D + k$, for $k = 1, \dots, s - 1$, 1_s is an $s \times 1$ vector with all elements unity, the operators \oplus and \otimes are defined in (2.1), D^* is the right circular design of D , and D^{**} is the right circular design of D^* , as given in Section 2.

Step 2. Treat all entries as numbers, and define

$$T_i = s^2 E_i + s F_i + G_i, \text{ for } i = 1, \dots, g.$$

Step 3. Combine T_i by column juxtaposition, and get $\bar{T} = (T_1, \dots, T_g)$.

Here is an illustrative example.

Example 4. Let $C = (c_1, c_2, c_3, c_4)$ be the $OA(9, 4, 3, 2)$ with entries from $GF(3)$ in Table 4. For $i = 1, 2, 3, 4$, create

$$E_i = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \\ 1 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \\ 2 & 2 & 2 \\ 2 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix} \oplus c_i, F_i = \begin{pmatrix} 0 & 0 & 0 \\ 2 & 0 & 1 \\ 1 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 1 \\ 1 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 1 \\ 1 & 0 & 2 \end{pmatrix} \oplus c_i, \text{ and } G_i = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 2 & 0 \\ 2 & 1 & 0 \end{pmatrix} \oplus c_i.$$

Treat all entries as numbers, and define $T_i = 9E_i + 3F_i + G_i$ for $i = 1, 2, 3, 4$. Then, we get an SGOA(81, 12, 27, 3) by taking $\bar{T} = (T_1, T_2, T_3, T_4)$, as shown in the left part of Table S.2 in the Supplementary Material.

For the resulting design \bar{T} in Algorithm 2, we have the following theorem.

Theorem 3. *The obtained \bar{T} in Algorithm 2 is an SGOA($s^2n_0, gs, s^3, 3$); that is, \bar{T} has the properties mentioned in Definition 1 with $n = s^2n_0, c = s$, and $t = 3$.*

Remark 3. In particular, if D is a difference scheme $D(s, h, s)$ in Algorithm 2, where $h \leq s$, then \bar{T} is an SGOA($s^2n_0, gh, s^3, 3$).

According to the proof of Theorem 3, any SGOA($s^2n_0, gs, s^3, 3$) generated by Algorithm 2 becomes an SGOA($s^2n_0, gs, s^2, 2$) after collapsing the factors into s^2 levels. In addition, the rows of this SGOA($s^2n_0, gs, s^2, 2$) can be partitioned into s parts, each of which is an SGOA($sn_0, gs, s^2, 2$). Furthermore, we can get SGOAs of strength 3 with a better three-dimensional space-filling property by taking C to be some specific OAs.

Theorem 4. *If C in Algorithm 2 is a regular OA($s^p, g_1, s, 2$) with $g_1 = 2^p - 1$, in which each generated column can be represented as the sum of q independent columns, where $2 \leq q \leq p$, then the resulting \bar{T} , an SGOA($s^{p+2}, g_1s, s^3, 3$), achieves a stratification on an $s \times s \times s$ grid in any three columns that do not belong to a same group, which implies that*

$$\delta = \left[\binom{g_1s}{3} - g_1 \binom{s}{3} \right] / \binom{g_1s}{3} = 1 - (s-2)(s-1) / \{(g_1s-2)(g_1s-1)\}. \quad (4.1)$$

We call the resulting design an improved SGOA of strength 3, owing to its better three-dimensional space-filling property. From (4.1), we can see that δ is quite close to one for a large g_1 . The following is an illustrative example.

Example 5 (Example 4 continued). Let C be the first three columns of the OA shown in Table 4, in which the third column can be represented as the sum of the first two columns. Then, we get an improved SGOA(81, 9, 27, 3), that is, the first nine columns of the SGOA(81, 12, 27, 3) shown in the left part of Table S.2 in the Supplementary Material. We can check that any three of its columns can be collapsed into an OA(81, 3, 3, 3), except for all three columns in T_1 , T_2 , or T_3 simultaneously. Thus, it achieves stratifications on $3 \times 3 \times 3$ grids in 81 of the 84 three dimensions; that is, $\delta = 96.43\%$.

Similarly, taking C in Algorithm 2 to be a regular OA(27, 7, 3, 2), OA(81, 15, 3, 2), OA(16, 3, 4, 2), and OA(25, 3, 5, 2) that satisfy the requirements in Theorem 4, we obtain the improved SGOA(243, 21, 27, 3), SGOA(729, 45, 27, 3), SGOA(256, 12, 64, 3), and SGOA(625, 15, 125, 3), respectively. The δ -values are 99.47%, 99.89%, 94.55%, and 93.41%, respectively. These designs all enjoy attractive three-dimensional space-filling properties.

Remark 4. In particular, if C is a regular OA(s^p , g_1 , s , 2) with $g_1 = 2^p - 1$ that satisfies the requirements in Theorem 4 and D is $(0, 1, \dots, s-1)^T$, a difference scheme $D(s, 1, s)$, then the resulting \bar{T} in Algorithm 2 is an OSOA(s^{p+2} , g_1 , s^3 , 3).

Remark 4 indicates that there is a close relationship between the improved SGOAs of strength 3 and OSOAs of strength 3. In fact, if we take one column from each

group of an improved SGOA($s^{p+2}, g_1s, s^3, 3$) and put these columns together, we get an OSOA($s^{p+2}, g_1, s^3, 3$). In addition, the resulting array has a better two-dimensional space-filling property than that of an ordinary OSOA of strength 3.

Table 8: Some SGOAs and OSOAs of strength 3.

C : OA($n_0, g, s, 2$)	\bar{T} : SGOA($s^2n_0, gs, s^3, 3$)	$\pi(\%)$	$\delta(\%)$	corr_{\max}^1	OSOA($s^2n_0, m, s^3, 3$) ²
OA(4, 3, 2, 2)	SGOA(16, 6, 8, 3)	80.00	100	0.190	OSOA(16, 4, 8, 3)
OA(8, 7, 2, 2)	SGOA(32, 14, 8, 3)	92.31	100	0.190	OSOA(32, 8, 8, 3)
OA(12, 11, 2, 2)	SGOA(48, 22, 8, 3)	95.24	100	0.190	OSOA(48, 12, 8, 3)
OA(16, 15, 2, 2)	SGOA(64, 30, 8, 3)	96.55	100	0.190	OSOA(64, 16, 8, 3)
OA(20, 19, 2, 2)	SGOA(80, 38, 8, 3)	93.70	100	0.190	OSOA(80, 20, 8, 3)
OA(24, 23, 2, 2)	SGOA(96, 46, 8, 3)	97.78	100	0.190	OSOA(96, 24, 8, 3)
OA(28, 27, 2, 2)	SGOA(112, 54, 8, 3)	98.11	100	0.190	OSOA(112, 28, 8, 3)
OA(32, 31, 2, 2)	SGOA(128, 62, 8, 3)	98.36	100	0.190	OSOA(128, 32, 8, 3)
OA(36, 35, 2, 2)	SGOA(144, 70, 8, 3)	98.55	100	0.190	OSOA(144, 36, 8, 3)
OA(40, 39, 2, 2)	SGOA(160, 78, 8, 3)	98.70	100	0.190	OSOA(160, 40, 8, 3)
OA(44, 43, 2, 2)	SGOA(176, 86, 8, 3)	98.82	100	0.190	OSOA(176, 44, 8, 3)
OA(48, 47, 2, 2)	SGOA(192, 94, 8, 3)	98.92	100	0.190	OSOA(192, 48, 8, 3)
OA(52, 51, 2, 2)	SGOA(208, 102, 8, 3)	99.01	100	0.190	OSOA(208, 52, 8, 3)
OA(56, 55, 2, 2)	SGOA(224, 110, 8, 3)	99.08	100	0.190	OSOA(224, 56, 8, 3)
OA(60, 59, 2, 2)	SGOA(240, 118, 8, 3)	99.15	100	0.190	OSOA(240, 60, 8, 3)
OA(64, 63, 2, 2)	SGOA(256, 126, 8, 3)	99.20	100	0.190	OSOA(256, 64, 8, 3)
OA(68, 67, 2, 2)	SGOA(272, 134, 8, 3)	99.25	100	0.190	OSOA(272, 68, 8, 3)
OA(72, 71, 2, 2)	SGOA(288, 142, 8, 3)	99.29	100	0.190	OSOA(288, 72, 8, 3)
OA(76, 75, 2, 2)	SGOA(304, 150, 8, 3)	99.33	100	0.190	OSOA(304, 76, 8, 3)
OA(80, 79, 2, 2)	SGOA(320, 158, 8, 3)	99.36	100	0.190	OSOA(320, 80, 8, 3)
OA(84, 83, 2, 2)	SGOA(336, 166, 8, 3)	99.39	100	0.190	OSOA(336, 84, 8, 3)
OA(88, 87, 2, 2)	SGOA(352, 174, 8, 3)	99.42	100	0.190	OSOA(352, 88, 8, 3)
OA(92, 91, 2, 2)	SGOA(368, 182, 8, 3)	99.45	100	0.190	OSOA(368, 92, 8, 3)
OA(96, 95, 2, 2)	SGOA(384, 190, 8, 3)	99.47	100	0.190	OSOA(384, 96, 8, 3)
OA(100, 99, 2, 2)	SGOA(400, 198, 8, 3)	99.49	100	0.190	OSOA(400, 100, 8, 3)
OA(9, 4, 3, 2)	SGOA(81, 12, 27, 3)	81.82	94.09	0.033	OSOA(81, 4, 27, 3)
OA(27, 13, 3, 2)	SGOA(243, 39, 27, 3)	94.74	98.58	0.033	OSOA(243, 10, 27, 3)
OA(81, 40, 3, 2)	SGOA(729, 120, 27, 3)	98.32	99.57	0.033	OSOA(729, 28, 27, 3)
OA(16, 5, 4, 2)	SGOA(256, 20, 64, 3)	84.21	92.63	0.015	OSOA(256, 8, 64, 3)
OA(25, 6, 5, 2)	SGOA(625, 30, 125, 3)	86.21	66.50	0.008	OSOA(625, 12, 125, 3)

¹ corr_{\max} represents the maximum correlation coefficient between any two distinct columns in one group; ²OSOA of strength 3 generated using the method in Liu and Liu (2015).

Table 8 lists some SGOAs of strength 3 obtained using Algorithm 2 and the cor-

responding OSOAs of strength 3 with the same run sizes; the OAs used are available in the library of OAs (<http://neilsloane.com/oadir/index.html>). Note that if $s = 2$, we have $\delta = 1$, which means that any three columns guarantee a stratification on an $s \times s \times s$ grid. Actually, SGOAs of strength 3 can be regarded as generalized versions of OSOAs of strength 3, where the proportion δ measures the degree of proximity of the three-dimensional space-filling property, and the proportion π characterizes the degree of proximity of the column orthogonality. As shown in Table 8, the values of π and δ are very close to one or just equal to one (for δ when $s = 2$), which means that these SGOAs of strength 3 have almost the same three-dimensional space-filling property and column orthogonality as those of the OSOAs of strength 3. Furthermore, the SGOAs of strength 3 have better space-filling properties in the sense of the stratifications on $s \times s^3$ and $s^3 \times s$ grids, with a large proportion π . At the same time, the values of corr_{\max} are very small, implying that even if any two columns in the same group are usually not column orthogonal, the correlation between them is acceptable. In addition, for $s = 2$, the SGOA of strength 3 with n runs accommodates $n/2 - 2$ columns, which is nearly twice the number ($n/4$) of the corresponding OSOA. For $s > 2$, they can have far more columns than the corresponding OSOAs do. For example, for a given run size 243, an OSOA of strength 3 can accommodate ten columns. Furthermore, it guarantees stratifications on 3×9 and 9×3 grids in any two dimensions, and a stratification on a $3 \times 3 \times 3$ grid in any three dimensions. The corresponding SGOA of strength 3 can accommodate 39 columns, and it guarantees stratifications on 3×9 and 9×3 grids in any two dimensions, and enjoys column orthogonality and stratifications

on 3×27 and 27×3 grids, with a large proportion 94.74%. Even if any two columns in the same group are usually not column orthogonal, the correlation between them is no larger than 0.033. In terms of the three-dimensional space-filling property, it enjoys stratifications on $3 \times 3 \times 3$ grids in a large proportion of 98.58%. Compared with the nine-level MNOA, the SGOA of strength 3 has better one-dimensional stratification, and can guarantee stratifications on 3×9 and 9×3 grids in any two dimensions. In contrast, the MNOA can only guarantee a stratification on a 3×3 grid in any two dimensions. Therefore, the SGOAs of strength 3 are more economical and suitable for computer experiments.

5. Conclusion

In this paper, we propose a new class of designs called SGOAs that enjoy attractive column orthogonality and space-filling properties in both two and three dimensions. Construction methods for this class of arrays based on both regular and nonregular designs are developed. The resulting designs have flexible run sizes that are not restricted to prime powers. At the same time, the methods are easy to implement.

Compared with MNOAs, the proposed SGOAs have flexible run sizes and better three-dimensional space-filling properties. The SGOAs have similar or better (in the case of strength 3) low-dimensional space-filling properties compared with those of the OSOAs, and can accommodate more factors. In addition, the SGOAs perform well in terms of column orthogonality, because they satisfy column orthogonality with large proportions. These desirable properties make SGOAs competitive designs for computer experiments.

Supplementary Material

The online Supplementary Material includes proofs of the theorems and two large tables.

Acknowledgments

The authors thank Professor Boxin Tang, Editor Hans-Georg Müller, an associate editor, and two referees for their valuable comments and suggestions. This work was supported by the National Natural Science Foundation of China (Grant Nos. 11771219, 11771220 and 11871288), National Ten Thousand Talents Program, and Tianjin Development Program for Innovation and Entrepreneurship. The first two authors contributed equally to this work. Min-Qian Liu is the corresponding author.

References

- Fang, K. T., Li, R. and Sudjianto, A. (2006). *Design and Modeling for Computer Experiments*. Chapman and Hall/CRC, New York.
- He, Y. Z. and Tang, B. (2013). Strong orthogonal arrays and associated Latin hypercubes for computer experiments. *Biometrika* **100**, 254–260.
- He, Y. Z. and Tang, B. (2014). A characterization of strong orthogonal arrays of strength three. *Ann. Statist.* **42**, 1347–1360.
- He, Y. Z., Cheng, C. S. and Tang, B. (2018). Strong orthogonal arrays of strength two plus. *Ann. Statist.* **46**, 457–468.

Hedayat, A. S., Sloane, N. J. A. and Stufken, J. (1999). *Orthogonal Arrays: Theory and Applications*. Springer, New York.

Liu, H. Y. and Liu, M. Q. (2015). Column-orthogonal strong orthogonal arrays and sliced strong orthogonal arrays. *Statist. Sinica* **25**, 1713–1734.

McKay, M. D., Beckman, R. J. and Conover, W. J. (1979). A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* **21**, 239–245.

Mukerjee, R., Sun, F. and Tang, B. (2014). Nearly orthogonal arrays mappable into fully orthogonal arrays. *Biometrika* **101**, 957–963.

Owen, A. B. (1992). Orthogonal arrays for computer experiments, integration and visualization. *Statist. Sinica* **2**, 439–452.

Tang, B. (1993). Orthogonal arrays based Latin hypercubes. *J. Amer. Statist. Assoc.* **88**, 1392–1397.

Zhou, Y. and Tang, B. (2019). Column-orthogonal strong orthogonal arrays of strength two plus and three minus. *Biometrika* **106**, 997–1004.

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

E-mail: 2120150092@mail.nankai.edu.cn

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

E-mail: jyyang@nankai.edu.cn

School of Statistics and Data Science, LPMC & KLMDASR, Nankai University, Tianjin

300071, China

E-mail: mqliu@nankai.edu.cn

Statistica Sinica