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CONSTRUCTION OF STRONG GROUP-ORTHOGONAL ARRAYS

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Abstract: Space-filling designs with low-dimensional stratifications are desirable choices for computer experiments. In addition, the column-orthogonality is an important property of designs for computer experiments, as it allows the estimates of the main effects in linear models to be uncorrelated with each other. Not much work has been done to study the space-filling designs with both properties. This paper proposes a new class of designs called strong group-orthogonal arrays whose columns can be partitioned into groups with the columns from different groups being column-orthogonal and enjoying attractive low-dimensional stratifications. Meanwhile, the whole arrays can be collapsed to fully orthogonal arrays which 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. Meanwhile, the proposed methods are easy to implement and do not require computer search.

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

1. Introduction

Computer experiments are being widely used in many fields in recent decades, and space-filling designs have been appropriate designs for computer experiments (Fang,

Li and Sudjianto (2006)). A space-filling design is a design that spreads its points in the design region uniformly, where the uniformity can be evaluated by some distance criteria 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. There have been a lot of approaches for constructing space-filling designs with good properties in low-dimensional projections using orthogonal arrays (OAs) or other arrays which can be collapsed into OAs, such as the SOAs and MNOAs mentioned below. 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 strong orthogonal arrays (SOAs) and Mukerjee, Sun and Tang (2014) proposed mappable nearly orthogonal arrays (MNOAs). Both arrays are better space-filling designs than those based on ordinary OAs. In addition to the space-filling property, the columnorthogonality is also a desirable property for the designs of computer experiments since it can guarantee that the estimates of the main effects are uncorrelated with each other when the polynomial modeling is considered.

Motivated by MNOAs and SOAs, in this paper we propose a new class of arrays called strong group-orthogonal arrays (SGOAs) whose columns 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 perform well in both space-filling property and column-orthogonality, and can accommodate large numbers of factors. To see the benefits of such an array, let us consider the four arrays

Table 1: The $OA(8,7)$	(7,2,2), OSOA(8,3,4,3)	(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	$5 \ 4 \ 1$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$1 \ 1 \ 1 \ 0 \ 0 \ 0 \ 1$	2 2 1	7 7 7	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

in Table 1, where the detailed definitions of these arrays will be introduced in Section 2. The column-orthogonal SOA((8, 3, 4, 3-), denoted as OSOA((8, 3, 4, 3-), constructed in Zhou and Tang (2019) can accommodate 3 factors, which achieves 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, which also holds for the SOA((8, 3, 8, 3)). The SOA((8, 3, 8, 3) is of 8-level and cannot guarantee the column-orthogonality. The SGOA((8, 6, 4, 2) constructed in this paper can accommodate 6 factors, each of 4 levels. It can guarantee stratifications on 2×4 and 4×2 grids and column-orthogonality in 12 out of all 15 two dimensions (80.00%) and stratifications on $2 \times 2 \times 2$ grids in 16 out of all 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 one, so it is a more economical choice.

Table 2: Properties of	of the $OSOA(8, 3, 4, 3 - $	$(\cdot), SOA(8,3,8,3)$	and $SGOA(8, 6, 4, 2)$.
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		Two-dimensional	Three-dimensional
Design	Column-orthogonality	stratification	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 OSOA(8, 3, 4, 3-). Correspondingly, an LHD based on the SGOA(8, 6, 4, 2) can be regarded as an intermediate between the ones based on the OA(8, 7, 2, 2) and SOA(8, 3, 8, 3), where the SOA(8, 3, 8, 3) is actually an LHD. According to Mukerjee, Sun and Tang (2014), the MNOA of 8 runs with 4 levels is not available, implying that SGOAs have more flexible run sizes than MNOAs. All these attractive properties make the SGOA(8, 6, 4, 2) a better choice for computer experiments.

This paper is organized as follows. Section 2 introduces the definitions and notation used in this paper. In Section 3, we propose the construction of SGOAs of strength 2. Section 4 devotes itself to the construction of 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, \ldots, s_m levels, denoted by OA $(n, m, s_1 \times \cdots \times s_m, t)$, if all possible level-combinations for any t columns occur with the same frequency. When all the s_j 's 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 $a = (a_1, \ldots, a_n)^T$ and $b = (b_1, \ldots, b_n)^T$ is defined as

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

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 0. 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 of *D* respectively, $1 \leq i, j \leq m$. A design is called column-orthogonal if any two columns of it 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 ($t \ge 2$) dimensions if the corresponding t columns of it 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 factorial effects of it are either combinatorial-orthogonal to each other or 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, ..., 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, ..., (j + 1)n/q - 1 for j = 0, 1, ..., 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 ith and jth 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

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

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

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 MNOA $\{n; (s^{\mu})^{\phi}, (p^{\mu})^{\phi}\}$, is an $n \times \mu \phi$ array whose $\mu \phi$ 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 OA(n, 2, s, 2);
- (iii) the whole design can be collapsed into an OA($n, \mu \phi, p, 2$), where $p \leq s$ and the s levels of a factor are collapsed into p levels by $\lfloor x/(s/p) \rfloor$ for $x = 0, 1, \ldots, s 1$, therein $\lfloor z \rfloor$ represents 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 $\{0, 1, \ldots, s^t - 1\}$ is called an SOA of strength t, denoted by SOA (n, m, s^t, t) , if any $n \times f$ submatrix, $1 \leq f \leq t$, can be collapsed into an OA $(n, f, s^{\mu_1} \times \cdots \times s^{\mu_f}, f)$ for any positive integers μ_1, \ldots, μ_f with $\mu_1 + \cdots + \mu_f = t$, where the s^t levels of a factor are collapsed into s^{μ_j} levels by $\lfloor x/s^{t-\mu_j} \rfloor$ for $x = 0, 1, \ldots, s^t - 1, 1 \leq j \leq f$. Furthermore, an $n \times m$ matrix with entries from $\{0, 1, \ldots, s^2 - 1\}$ is called an SOA of strength 2+, denoted by SOA $(n, m, s^2, 2+)$, if any submatrix of two columns can be collapsed into an OA $(n, 2, s^2 \times s, 2)$ and an OA $(n, 2, s \times s^2, 2)$. An $n \times m$ matrix with entries from $\{0, 1, \ldots, s^2 - 1\}$ is called an SOA of $(n, m, s^2, 3-)$, if any submatrix of two columns can be collapsed into an OA $(n, 2, s \times s^2, 2)$, and any submatrix of three columns can be collapsed into an OA $(n, 2, s \times s^2, 2)$, and any submatrix of three columns can be collapsed into an OA $(n, 2, s \times s^2, 2)$.

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 $(n, m, s^2, 3-)$.

Pre-collapsing	Post-collapsing
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c c}\hline \hline A_1 & A_2 & A_3 & A_4 \\ \hline \end{array}$
0 0 0 4 4 4 4 4 4 8 8 8	$0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 1 \ 1 \ 2 \ 2 \ 2$
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 \ $
4 4 4 4 4 4 8 8 8 0 0 0	$1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 0$
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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
8 8 8 4 4 4 0 0 0 4 4 4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
2 3 7 3 7 2 3 7 2 7 2 3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
2 3 7 7 2 3 7 2 3 3 7 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
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	$1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 1 \ 2 \ 0 \ 1$
7 2 3 2 3 7 7 2 3 7 2 3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
7 2 3 3 7 2 2 3 7 3 7 2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
7 2 3 7 2 3 3 7 2 2 3 7	$\begin{array}{ cccccccccccccccccccccccccccccccccccc$
1 6 5 1 6 5 1 6 5 1 6 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
1 6 5 5 1 6 5 1 6 6 5 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$1 \ 6 \ 5 \ 6 \ 5 \ 1 \ 6 \ 5 \ 1 \ 5 \ 1 \ 6$	$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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
651651516165	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

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

Before giving the definition of the new class of SGOAs, let us first look at the array in the left part of Table 3. It has 12 columns, where each of them is populated by 9 levels. If we partition these columns into 4 disjoint groups of 3 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 $OA(27, 2, 9 \times 3, 2)$ by different collapsing methods;
- (iii) any three distinct columns from two different groups can be collapsed into an OA(27, 3, 3, 3).

Definition 1. A strong group-orthogonal array (SGOA) of strength t, denoted by SGOA (n, gc, s^t, t) , is an $n \times gc$ matrix with entries from $\{0, 1, \dots, s^t - 1\}$ which 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 $OA(n, 2, s^{t-1} \times s, 2)$ by 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 $OA(n, 2, s^t \times s, 2)$ by 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). Since an SGOA(n, gc, s^t, t) with $t \ge 2$ can be collapsed into an OA(n, gc, s, 2), then 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. It is worth noting that the strength t of an SGOA is an index to measure the space-filling

property in two dimensions. The larger t is, the more space-filling an SGOA is in two dimensions. For an SGOA $(n, gc, s^2, 2)$, if c = 1 (i.e., each group of it has only one column), it becomes an OSOA $(n, g, s^2, 2+)$. Thus, the SGOA of strength 2 can be seen as a generalization of the OSOA of strength 2+. We can also see that 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 OA $(n, 2, s \times s^t, 2)$'s and OA $(n, 2, s^t \times s, 2)$'s. For an SGOA (n, gc, s^t, t) with $t \ge 2$, we use π to denote the proportion of 2-tuples which 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 3-tuples which 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 can see that the δ -value of an SGOA is often larger than δ_0 , and under some conditions, we can obtain some 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. As the general method may not be easy to understand without examples, we first 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
L			

present two examples to illustrate the main idea.

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

$$A_{i} = \begin{pmatrix} c_{i} & c_{i} & c_{i} \\ c_{i} & c_{i}+1 & c_{i}+2 \\ \vdots & \vdots & \vdots \\ c_{i} & c_{i}+2 & c_{i}+1 \end{pmatrix} \text{ and } B_{i} = \begin{pmatrix} c_{i} & c_{i} & c_{i} \\ \vdots & \vdots & \vdots \\ c_{i}+2 & c_{i} & c_{i}+1 \\ \vdots & \vdots \\ c_{i}+1 & c_{i} & c_{i}+2 \end{pmatrix},$$

where $\dot{+}$ 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 can get 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 the 3-tuples, we can find that \tilde{T} achieves stratifications on $3 \times 3 \times 3$ grids in 180 out of all 220 three dimensions, i.e. $\delta = 81.82\%$, which is much larger than $\delta_0 = 49.09\%$.

			/ I	
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

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

Example 2. We now construct an SGOA(64, 20, 16, 2). Let $C = (c_1, \ldots, c_5)$ be an

OA(16, 5, 4, 2) with entries from GF(4) as shown in Table 5. For $i = 1, \ldots, 5$, define

$$A_{i} = \begin{pmatrix} c_{i} & c_{i} & c_{i} & c_{i} \\ c_{i} & c_{i} + 1 & c_{i} + 2 & c_{i} + 3 \\ c_{i} & c_{i} + 2 & c_{i} + 3 & c_{i} + 1 \\ c_{i} & c_{i} + 3 & c_{i} + 1 & c_{i} + 2 \end{pmatrix} \text{ and } B_{i} = \begin{pmatrix} c_{i} & c_{i} & c_{i} & c_{i} \\ \vdots & \vdots & \vdots & \vdots \\ c_{i} + 3 & c_{i} + 1 & c_{i} + 2 \\ \vdots & \vdots & \vdots & \vdots \\ c_{i} + 1 & c_{i} & c_{i} + 2 & c_{i} + 3 \\ \vdots & \vdots & \vdots & \vdots \\ c_{i} + 2 & c_{i} & c_{i} + 3 & c_{i} + 1 \end{pmatrix}$$

where $\dot{+}$ is the addition defined on GF(4). Treat all entries as numbers and create $T_i = 4A_i + B_i$ for i = 1, ..., 5. We can 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 they can be collapsed into an OA(64, 2, 4 \times 16, 2) and an OA(64, 2, 16 \times 4, 2), the proportion π takes 84.21%. We can also check that any three

distinct columns from two different groups of \tilde{T} can be collapsed into an OA(64, 3, 4, 3) with $\delta_0 = 480/1140 = 42.11\%$. Furthermore, by checking all the 3-tuples, we can find that \tilde{T} achieves stratifications on $4 \times 4 \times 4$ grids in 960 out of all 1140 three dimensions, i.e. $\delta = 84.21\%$.

Next, we present the construction of the 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 $C = (c_1, \ldots, c_g)$ be an OA $(n_0, g, s, 2)$ with entries from GF(s) and D be a difference scheme D(s, s, s). For $i = 1, \ldots, g$, 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

$$T_i = sA_i + B_i$$
, for $i = 1, ..., g$.

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

For the resulting design, we have

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

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

According to Remark 1, we can see that 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 SGOA($n, gc, s^2, 2$) and put these columns together, we can get an OSOA($n, g, s^2, 2+$). In this sense, SGOAs of strength 2 can be regarded as a generalized version of the OSOAs of strength 2+, where the proportion π can measure the degree of proximity in terms of both column-orthogonality and 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 $0, 1, \ldots, s - 1$ 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 slevels as well, which 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 can get some SGOAs with large δ -values, which means that the resulting designs enjoy a better space-filing 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 , i.e. $\delta = \pi$.

From Theorem 2, there are many SGOAs enjoying 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, where symbol \sharp 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, and symbol \ddagger means that if *C* is a saturated regular design, 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 1, implying that the resulting designs enjoy attractive space-filling properties and column-orthogonality.

Comparisons among SGOAs, MNOAs in Mukerjee, Sun and Tang (2014), SOAs in He, Cheng and Tang (2018), Liu and Liu (2015) and Zhou and Tang (2019) are listed in Table 7.

As we have discussed, SGOAs of strength 2 can be regarded as a generalized version of the OSOAs of strength 2+, where the proportion π can measure the degree of proximity in terms of both column-orthogonality and two-dimensional space-filling property. From Table 7, we can see that the values of π are very close to 1, which means

$C: OA(n_0, g, s, 2)$ $\bar{T}: SGOA(sn_0, gs, s^2, 2)$ $\pi(\%)$ $OA(4, 3, 2, 2)$ $SGOA(8, 6, 4, 2)$ 80.00 $OA(4, 3, 2, 2)$ $SGOA(16, 14, 4, 2)$ 92.31 $OA(12, 11, 2, 2)$ $SGOA(24, 22, 4, 2)$ 95.24 $OA(16, 15, 2, 2)$ $SGOA(32, 30, 4, 2)$ 97.30 $OA(20, 19, 2, 2)$ $SGOA(40, 38, 4, 2)$ 97.30 $OA(24, 23, 2, 2)$ $SGOA(46, 62, 4, 2)$ 97.78 $OA(28, 27, 2, 2)$ $SGOA(64, 62, 4, 2)$ 98.51 $OA(32, 31, 2, 2)$ $SGOA(64, 62, 4, 2)$ 98.55 $OA(36, 35, 2, 2)$ $SGOA(72, 70, 4, 2)$ 98.55 $OA(40, 39, 2, 2)$ $SGOA(80, 78, 4, 2)$ 98.82 $OA(44, 43, 2, 2)$ $SGOA(104, 102, 4, 2)$ 98.82 $OA(44, 47, 2, 2)$ $SGOA(104, 102, 4, 2)$ 99.01 $OA(55, 55, 2, 2)$ $SGOA(112, 110, 4, 2)$ 99.01 $OA(66, 59, 2, 2)$ $SGOA(112, 110, 4, 2)$ 99.02 $OA(66, 57, 2, 2)$ $SGOA(120, 118, 4, 2)$ 99.25 $OA(64, 63, 2, 2)$ $SGOA(126, 152, 150, 4, 2)$ 99.25 $OA(72, 71, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.33 $OA(80, 79, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.33 $OA(80, 79, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.39 $OA(84, 83, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.39 $OA(84, 83, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.39 $OA(84, 83, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.39 $OA(84, 83, 2, 2)$ $SGOA(160, 158, 4, 2)$ 99.39 $OA(84, 83, 2, 2)$ $SGOA(160, 158, 4, 2)$
$\begin{array}{c ccccc} OA(8,7,2,2) & SGOA(16,14,4,2)\sharp \ddagger & 92.31 \\ OA(12,11,2,2) & SGOA(24,22,4,2)\sharp & 95.24 \\ OA(16,15,2,2) & SGOA(32,30,4,2)\sharp \ddagger & 96.55 \\ OA(20,19,2,2) & SGOA(40,38,4,2)\sharp & 97.30 \\ OA(24,23,2,2) & SGOA(48,46,4,2)\sharp & 97.78 \\ OA(28,27,2,2) & SGOA(56,54,4,2)\sharp & 98.11 \\ OA(32,31,2,2) & SGOA(64,62,4,2)\sharp & 98.36 \\ OA(36,35,2,2) & SGOA(64,62,4,2)\sharp & 98.55 \\ OA(40,39,2,2) & SGOA(88,86,4,2)\sharp & 98.82 \\ OA(44,43,2,2) & SGOA(88,86,4,2)\sharp & 98.82 \\ OA(44,43,2,2) & SGOA(104,102,4,2)\sharp & 99.01 \\ OA(52,51,2,2) & SGOA(112,110,4,2)\sharp & 99.01 \\ OA(56,55,2,2) & SGOA(112,110,4,2)\sharp & 99.01 \\ OA(64,63,2,2) & SGOA(120,118,4,2)\sharp & 99.15 \\ OA(64,63,2,2) & SGOA(128,126,4,2)\sharp & 99.25 \\ OA(64,63,2,2) & SGOA(166,132,4,2)\sharp & 99.25 \\ OA(72,71,2,2) & SGOA(160,158,4,2)\sharp & 99.33 \\ OA(80,79,2,2) & SGOA(160,158,4,2)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(160,158,4,2)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42,42,42)\sharp & 99.45 \\ \end{array}$
$\begin{array}{c ccccc} OA(8,7,2,2) & SGOA(16,14,4,2)\sharp \ddagger & 92.31 \\ OA(12,11,2,2) & SGOA(24,22,4,2)\sharp & 95.24 \\ OA(16,15,2,2) & SGOA(32,30,4,2)\sharp \ddagger & 96.55 \\ OA(20,19,2,2) & SGOA(40,38,4,2)\sharp & 97.30 \\ OA(24,23,2,2) & SGOA(48,46,4,2)\sharp & 97.78 \\ OA(28,27,2,2) & SGOA(56,54,4,2)\sharp & 98.11 \\ OA(32,31,2,2) & SGOA(64,62,4,2)\sharp & 98.36 \\ OA(36,35,2,2) & SGOA(64,62,4,2)\sharp & 98.55 \\ OA(40,39,2,2) & SGOA(88,86,4,2)\sharp & 98.82 \\ OA(44,43,2,2) & SGOA(88,86,4,2)\sharp & 98.82 \\ OA(44,43,2,2) & SGOA(104,102,4,2)\sharp & 99.01 \\ OA(52,51,2,2) & SGOA(112,110,4,2)\sharp & 99.01 \\ OA(56,55,2,2) & SGOA(112,110,4,2)\sharp & 99.01 \\ OA(64,63,2,2) & SGOA(120,118,4,2)\sharp & 99.15 \\ OA(64,63,2,2) & SGOA(128,126,4,2)\sharp & 99.25 \\ OA(64,63,2,2) & SGOA(166,132,4,2)\sharp & 99.25 \\ OA(72,71,2,2) & SGOA(160,158,4,2)\sharp & 99.33 \\ OA(80,79,2,2) & SGOA(160,158,4,2)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(160,158,4,2)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.39 \\ OA(84,83,2,2) & SGOA(166,164,42)\sharp & 99.36 \\ OA(84,83,2,2) & SGOA(166,164,42,42,42)\sharp & 99.45 \\ \end{array}$
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$\begin{array}{cccccccc} OA(64,63,2,2) & SGOA(128,126,4,2) \sharp \ddagger & 99.20 \\ OA(68,67,2,2) & SGOA(136,132,4,2) \sharp & 99.25 \\ OA(72,71,2,2) & SGOA(144,142,4,2) \sharp & 99.29 \\ OA(76,75,2,2) & SGOA(152,150,4,2) \sharp & 99.33 \\ OA(80,79,2,2) & SGOA(160,158,4,2) \sharp & 99.36 \\ OA(84,83,2,2) & SGOA(168,166,4,2) \sharp & 99.39 \\ OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \\ \end{array}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{ccccccc} OA(72,71,2,2) & SGOA(144,142,4,2) \sharp & 99.29 \\ OA(76,75,2,2) & SGOA(152,150,4,2) \sharp & 99.33 \\ OA(80,79,2,2) & SGOA(160,158,4,2) \sharp & 99.36 \\ OA(84,83,2,2) & SGOA(168,166,4,2) \sharp & 99.39 \\ OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \\ \end{array}$
$\begin{array}{cccc} OA(76,75,2,2) & SGOA(152,150,4,2) \sharp & 99.33 \\ OA(80,79,2,2) & SGOA(160,158,4,2) \sharp & 99.36 \\ OA(84,83,2,2) & SGOA(168,166,4,2) \sharp & 99.39 \\ OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \\ \end{array}$
$\begin{array}{cccc} OA(80,79,2,2) & SGOA(160,158,4,2) \sharp & 99.36 \\ OA(84,83,2,2) & SGOA(168,166,4,2) \sharp & 99.39 \\ OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \\ \end{array}$
$\begin{array}{cccc} OA(84,83,2,2) & SGOA(168,166,4,2) \sharp & 99.39 \\ OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \end{array}$
$\begin{array}{ccc} OA(88,87,2,2) & SGOA(176,174,4,2) \sharp & 99.42 \\ OA(92,91,2,2) & SGOA(184,182,4,2) \sharp & 99.45 \end{array}$
OA(92, 91, 2, 2) $SGOA(184, 182, 4, 2)$ 99.45
OA(100, 99, 2, 2) $SGOA(200, 198, 4, 2)$ 99.49
$OA(9, 4, 3, 2)$ SGOA(27, 12, 9, 2) \sharp 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

Table 6: Some SGOAs of strength 2.

that these SGOAs of strength 2 have almost the same desirable column-orthogonality and two-dimensional space-filling property as the OSOAs of strength 2+. Besides, they can accommodate *s* times as many columns as the latter ones and have a better performance in three dimensions. The OSOAs of strength 2 are better than SGOAs of strength 2 in terms of column-orthogonality, and can accommodate more (or equally many) factors, while the SGOAs of strength 2 enjoy better two- and three-dimensional

			$(n, gs, s^2, 2)$	MNG	DA ¹	$SOA(2+)^2$	$OSOA(2)^3$	OSOA($p)^4$
s	n	$\pi(\%)$	gs	$\bar{\pi}(\%)$	$\mu\phi$	m	m	m	p
2	8	80.00	6	—	_	—	—	3	3-
2	$24,\!40,\!48$	$\frac{n-4}{n-3}$	n-2	—	—	—	_	n/2 - 1	3-
	56,72,80								
	88,96,104								
	112,120								
	$136,\!144,\!152$								
	160, 168, 176								
	184,192,200								
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+

Table 7: Comparisons	among SGOAs	of strength 2.	MNOAs.	. SOAs and OSOAs.
rasie ii companioni		or serongen =		

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.

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. Besides, SGOAs are particularly useful when the 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 while such MNOAs are not avail-

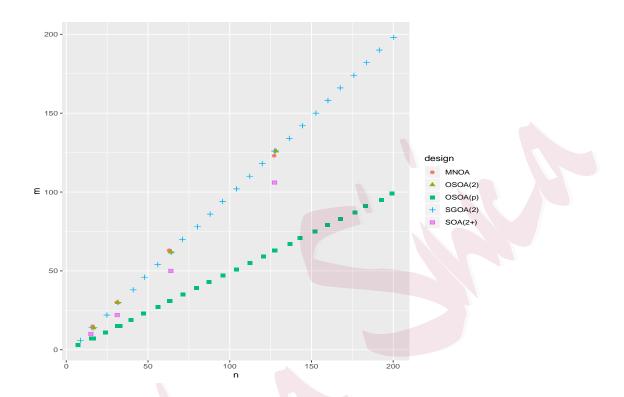


Figure 1: Comparison of SGOAs of strength 2 with some related designs for s = 2.

able. All these desirable properties ensure the SGOAs to be 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 corresponding type with n runs and m factors. We can see that SGOAs have flexible run sizes and can accommodate large number 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 that of the SGOAs of strength 2. With Definition 1, we know that an SGOA of strength 3, denoted by SGOA $(n, gc, s^3, 3)$, is an $n \times gc$ matrix with entries from $\{0, 1, \ldots, s^3 - 1\}$ which 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 $OA(n, 2, s \times s^2, 2)$ and an $OA(n, 2, s^2 \times s, 2)$ by different collapsing methods;
- (ii) any two columns from different groups are column-orthogonal and they can be collapsed into an $OA(n, 2, s \times s^3, 2)$ and an $OA(n, 2, s^3 \times s, 2)$ by 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 $\overline{T} = (T_1, T_2, T_3, T_4)$ 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 × 9, 2) and an OA(81, 2, 9 × 3, 2). Any two columns from different groups are column-orthogonal and they can be collapsed into an OA(81, 2, 3 × 27, 2) and an OA(81, 2, 27 × 3, 2), thus we have $\pi = 81.82\%$. And the maximum correlation coefficient between any two distinct columns from one group is 0.033, implying that \overline{T} is nearly column-orthogonal. Collapsing each factor into 3 levels, we can 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 of it form an OA(81, 3, 3, 3). Thus, \overline{T} achieves stratifications on $3 \times 3 \times 3$ grids in at least 108 out of all 220 three dimensions, i.e. $\delta_0 = 49.09\%$. In fact, by checking all the 3-tuples, we find that \overline{T} achieves stratifications on $3 \times 3 \times 3$ grids in 207 out of all 220 three dimensions, i.e.

 $\delta = 94.09\%$. Thus, the design enjoys attractive space-filling properties in both two and three dimensions and near column-orthogonality.

Now, let us 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 $C = (c_1, \ldots, c_g)$ be an $OA(n_0, g, s, 2)$ with entries from GF(s) and D be a difference scheme D(s, s, s). For $i = 1, \ldots, g$, 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 $k = 1, ..., s - 1, 1_s$ 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

$$T_i = s^2 E_i + sF_i + G_i$$
, for $i = 1, \dots, g$.

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

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

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

Table 4. For i = 1, 2, 3, 4, create

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

For the resulting design \overline{T} in Algorithm 2, we have

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

Remark 3. In particular, if D is a difference scheme D(s, h, s) in Algorithm 2, where $h \leq s$, then \overline{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. And 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 $g_1 = 2^p - 1$ whose each generated column can be represented as the sum of q independent columns, where $2 \le q \le p$, then the resulting \overline{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

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

We call the resulting design an improved SGOA of strength 3 due to its better three-dimensional space-filling property. From (4.1), we can see that δ is quite close to 1 for a large g_1 . Let us see an illustrative example.

Example 5 (Example 4 continued). Let C be the first three columns of the OA shown in Table 4, whose third column can be represented as the sum of the first two columns. Then we can get an improved SGOA(81, 9, 27, 3), that is, the first 9 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 columns of it 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 out of all 84 three dimensions, i.e. $\delta = 96.43\%$.

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) which satisfy the requirements in Theorem 4, we can 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. All these designs 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 $(0, 1, ..., s - 1)^T$, a difference scheme D(s, 1, s), then the resulting \overline{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 can 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 an ordinary OSOA of strength 3.

Table 8 lists some SGOAs of strength 3 obtained through Algorithm 2 and the corresponding OSOAs of strength 3 with the same run sizes, where the OAs we 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 a generalized version of the OSOAs of strength 3, where the proportion δ can measure the degree of proximity of the three-dimensional space-filling property and the proportion π can characterize the degree of proximity of the column-orthogonality. As shown in Table 8, the values of π and δ are very close to 1 or just equal to 1 (for δ when s = 2), which means that these SGOAs of strength 3 have almost the same three-dimensional 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 . Meanwhile, the values of corr_{max} are very small, implying that even if any two columns in a same

C: $OA(n_0, g, s, 2)$	\overline{T} : SGOA $(s^2n_0, gs, s^3, 3)$	$\pi(\%)$	$\delta(\%)$	$\operatorname{corr}_{\max}^{1}$	$OSOA(s^2n_0, m, s^3, 3)^2$
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)

Table 8: Some SGOAs and OSOAs of strength 3.

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

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 can accommodate n/2 - 2 columns which is nearly twice of the ones (n/4) of the corresponding OSOA. For s > 2, they can have much more columns than the corresponding OSOAs. For example, for a given run size 243, an OSOA of strength 3 can accommodate 10 columns, and 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 a 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 98.58%. Compared with the 9-level MNOA, the SGOA of strength 3 has a better one-dimensional stratification and can guarantee stratifications on 3×9 and 9×3 grids in any two dimensions. Therefore, the SGOAs of strength 3 are more economical and suitable for computer experiments.

5. Concluding Remarks

In this paper, we propose a new class of designs called SGOAs, which 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 which are not restricted to prime powers. Meanwhile, the methods are easy to implement and do not require computer search.

Compared with the MNOAs, the proposed SGOAs have flexible run sizes and better

three-dimensional space-filling properties. The SGOAs have similar or even better (in the case of strength 3) low-dimensional space-filling properties compared with the OSOAs while they can accommodate more factors than the latter ones. In addition, the SGOAs perform well in column-orthogonality, as they satisfy column-orthogonality with large proportions. All these desirable properties make SGOAs competitive designs for computer experiments.

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