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A simple approach to constructing quasi-Sudoku-based sliced space-filling designs

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Abstract Sliced Sudoku-based space-filling designs and, more generally, quasi-sliced orthogonal array-based space-filling designs are useful experimental designs in several contexts, including computer experiments with categorical in addition to quantitative inputs and cross-validation. Here, we provide a straightforward construction of doubly orthogonal quasi-Sudoku Latin squares which can be used to generate quasi-sliced orthogonal arrays and, in turn, sliced space-filling designs which achieve uniformity in one- and two-dimensional projections for the full design and uniformity in two-dimensional projections for each slice. These constructions are very practical to implement and yield a spectrum of design sizes and numbers of factors not currently broadly available.

Keywords Computer experiments · Space-filling designs · Sudoku · Sliced experimental designs

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1 Introduction

In the popular game Sudoku, players are presented with a nine-by-nine array, divided into nine three-by-three subsubarrays, and partially filled with the numbers 1 through 9. The goal is to fill the nine-by-nine array with the numbers 1 through 9 so that each row, column, and three-by-three subarray contains no repeated numbers. See a starting and completed Sudoku square in Fig. 1 (USA Today 2013).

Sets of (completed) Sudoku squares, as well as generalizations thereof, can be used to construct sliced space-filling designs achieving uniformity in both one- and two-dimensional projections for both the complete design and each subdesign, or slice (Xu et al. 2011). Sliced space-filling designs are experimental designs which can be partitioned into groups of subdesigns, so that both the full design and each subdesign achieve some type of uniformity (Qian and Wu 2009). These types of designs are broadly useful for collecting data from computer experiments, large and time-consuming mathematical codes used to model real-world systems such as the climate or a component in an engineering design problem. Sliced space-filling designs are particularly useful for computer experiments with qualitative and quantitative inputs (Qian and Wu 2009), multiple levels of accuracy (Haaland and Qian 2010), and cross-validation problems in the context of computer experiments (Zhang and Qian 2013). Sudoku-based sliced space-filling designs were introduced in Xu et al. (2011) and a construction was given using doubly orthogonal Sudoku squares, whose complete arrays are orthogonal and whose subarrays are orthogonal after a projection. In Xu et al. (2011), doubly orthogonal Sudoku squares were constructed using the techniques developed in Pedersen and Vis (2009) along with a subfield projection.

Here, we give a straightforward construction for doubly orthogonal quasi-Sudoku squares from sets of orthogonal Latin squares. These constructions are relatively well described and available for a broad range of sizes (Colbourn and Dinitz 2006; Keedwell and Dénes 2015; Raghavarao 1971). A similar technique has been used by Li et al. (2015) to construct sliced orthogonal arrays of composite order from smaller orthogonal arrays, as well as constructions incorporating difference matrices. See also Ai et al. (2014) and Qian and Wu (2009) for related constructions. We give more details of the Li et al. (2015) construction techniques in Sect. 5 and comment on the comparisons and differences. However, one theoretical difference is that the constructions given in the current paper result in doubly orthogonal quasi-Sudoku Latin squares,

			7	**3**	**5**	**8**	**2**	
8				**1**				**5**
				2	**6**		**1**	
	8	**1**		**7**				**9**
	6			**9**			**5**	
9				**5**		**3**	**8**	
	3		**1**	**4**				
4				**6**				**3**
	9	**2**	**3**	**8**	**7**			

1	4	9	**7**	**3**	**5**	**8**	**2**	6
8	2	6	9	**1**	4	7	3	**5**
3	5	7	8	**2**	**6**	9	**1**	4
5	**8**	**1**	2	**7**	3	4	6	**9**
2	**6**	3	4	**9**	8	1	**5**	7
9	7	4	6	**5**	1	**3**	**8**	2
7	**3**	5	**1**	**4**	2	6	9	8
4	1	8	5	**6**	9	2	7	**3**
6	**9**	**2**	**3**	**8**	**7**	5	4	1

Fig. 1 A starting and completed Sudoku square USA Today 2013

with the doubly orthogonal Sudoku property leading to a straightforward verification that the corresponding orthogonal arrays may be partitioned into slices, which after an appropriate projection corresponds to asymmetric orthogonal arrays. Given that the "base ingredients" are orthogonal Latin squares, these new constructions deliver a wider class of designs.

The remainder of this article is organized as follows. Section 2 provides notation and definitions which will be used throughout. Section 3 provides a construction for sets of pairwise doubly orthogonal quasi-Sudoku Latin squares which is based on sets of orthogonal Latin squares. Section 4 illustrates the presented techniques with an example. Section 5 notes the connection with quasi-sliced asymmetric orthogonal arrays. Finally, Sect. 6 reviews the construction of Sudoku-based sliced space-filling designs from Xu et al. (2011).

2 Notation and definitions

Let $[n] = \{0, 1, \ldots, n-1\}$ and $A = [A(i, j)]$ be a Latin square of order n; that is, an $n \times n$ array in which each of the entries in a set N (usually $[n]$) of size n occurs once in every row and once in every column. Two Latin squares $A = [A(i, j)]$ and $B = [B(i, j)]$, of the same order, are said to be orthogonal if, when we superimpose one on top of the other, the arrays contain each of the n^2 ordered pairs (x, y), $x, y \in N$ exactly once. It is useful to note that A and B are orthogonal if and only if for all $p, q, s, t \in N$,

$$A(p, q) = A(s, t) \Longrightarrow B(p, q) \neq B(s, t).$$

Let $A = [A(i, j)]$ and $B = [B(i, j)]$ be two orthogonal Latin squares of order n. For $n = s^2$, let Π denote a projection from N to $[s]$, $\Pi : N \to [s]$, and let $\mathcal{O} = \{(\Pi(A(i, j)), \Pi(B(i, j))) \mid i, j \in N\}$. We may think of $\mathcal{O}$ as an $n \times n$ array obtained by superimposing $\Pi(A)$ and $\Pi(B)$. The Latin squares A and B are said to be doubly orthogonal if there exists a projection Π such that $\mathcal{O}$ can be partitioned into $s \times s$ subarrays with the cells of each subarray containing the s^2 ordered pairs (x, y), $0 \leq x, y \leq s-1$. For $n = rs$, let Π_r denote a projection from N to $[r]$, $\Pi_r : N \to [r]$, let Π_s denote a projection from N to $[s]$, $\Pi_s : N \to [s]$, and $\mathcal{O} = \{(\Pi_r(A(i, j)), \Pi_s(B(i, j))) \mid i, j \in N\}$. The Latin squares A and B are said to be doubly orthogonal if there exist projections Π_r and Π_s, such that $\mathcal{O}$ can be partitioned into $r \times s$ subarrays with the cells of each subarray containing the rs ordered pairs (x, y) where $0 \leq x \leq r-1$ and $0 \leq y \leq s-1$.

An $m^2 \times m^2$ array is said to be a Sudoku Latin square, on the set X of size m^2, if it is a Latin square and we can label the rows by (p, s), $0 \leq p, s \leq m-1$ and columns by (q, t), $0 \leq q, t \leq m-1$, such that for each p and q the subarray defined by the cells

$$((p, s), (q, t)), \quad 0 \leq s, t \leq m-1$$

A_1

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

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

B_1

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

A_2

0	1	2
1	2	0
2	0	1

B_2

0	1	2
2	0	1
1	2	0

Fig. 2 The three (pairwise) orthogonal Latin squares of order 4 and the two orthogonal Latin squares of order 3

contains each entry of X precisely once. An $mn \times mn$ array is said be a quasi-Sudoku Latin square, on the set X of order mn, if it is a Latin square and we can label the rows by (p, s), $0 \leq p \leq m-1$, $0 \leq s \leq n-1$ and columns (q, t), $0 \leq q \leq n-1$, $0 \leq t \leq m-1$, such that for each p and q the subarray defined by the cells

$$((p, s), (q, t)), \quad 0 \leq s \leq n-1, \quad 0 \leq t \leq m-1$$

contains each entry of X precisely once. Two Sudoku Latin squares or quasi-Sudoku Latin squares are orthogonal (doubly orthogonal) if they are orthogonal (doubly orthogonal) Latin squares.

3 Construction of doubly orthogonal quasi-Sudoku Latin squares

Here, we construct quasi-Sudoku Latin squares which are doubly orthogonal using sets of (pairwise) orthogonal Latin squares. This is done by first using a direct product construction to construct orthogonal quasi-Sudoku Latin squares and then showing that they are doubly orthogonal.

For the remainder of this section, we will take A_1 and A_2 to be two Latin squares of order m and n, respectively. We can construct a new Latin square of order mn by taking the direct product, $A_1 \otimes A_2$, of A_1 with A_2, where $(A_1(p, q), A_2(s, t))$ is the element in row $np + s$ and column $nq + t$ of $A_1 \otimes A_2$, $0 \leq p, q \leq m-1$ and $0 \leq s, t \leq n-1$. Label the rows of $A_1 \otimes A_2$ as (p, s) and the columns of $A_1 \otimes A_2$ as (q, t). For fixed p and q, the subarray defined by the set of cells $\{((p, s), (q, t)) \mid 0 \leq s, t \leq n-1\}$ is then isomorphic to A_2.

The next proposition attests that orthogonality is maintained under the direct product. For a proof, see Keedwell and Dénes (2015), p 427.

Proposition 1 *If A_1 and B_1 are orthogonal Latin squares of order m, and A_2 and B_2 are orthogonal Latin squares of order n, then $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are orthogonal Latin squares of order mn.*

An example of orthogonal Latin squares $A_1 \otimes A_2$ and $B_1 \otimes B_2$, constructed using the orthogonal Latin squares shown in Fig. 2, is described in Sect. 4 and shown in Fig. 3.

Proposition 2 *If A_1 and B_1 are orthogonal Latin squares of order m, and A_2 and B_2 are orthogonal Latin squares of order n, then $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are doubly orthogonal quasi-Sudoku Latin squares of order mn.*

$A_1 \otimes A_2$

	00	01	02	10	11	12	20	21	22	30	31	32
00	00	01	02	10	11	12	20	21	22	30	31	32
01	01	02	00	11	12	10	21	22	20	31	32	30
02	02	00	01	12	10	11	22	20	21	32	30	31
10	10	11	12	00	01	02	30	31	32	20	21	22
11	11	12	10	01	02	00	31	32	30	21	22	20
12	12	10	11	02	00	01	32	30	31	22	20	21
20	20	21	22	30	31	32	00	01	02	10	11	12
21	21	22	20	31	32	30	01	02	00	11	12	10
22	22	20	21	32	30	31	02	00	01	12	10	11
30	30	31	32	20	21	22	10	11	12	00	01	02
31	31	32	30	21	22	20	11	12	10	01	02	00
32	32	30	31	22	20	21	12	10	11	02	00	01

$B_1 \otimes B_2$

	00	01	02	10	11	12	20	21	22	30	31	32
00	00	01	02	10	11	12	20	21	22	30	31	32
01	02	00	01	12	10	11	22	20	21	32	30	31
02	01	02	00	11	12	10	21	22	20	31	32	30
10	20	21	22	30	31	32	00	01	02	10	11	12
11	22	20	21	32	30	31	02	00	01	12	10	11
12	21	22	20	31	32	30	01	02	00	11	12	10
20	30	31	32	20	21	22	10	11	12	00	01	02
21	32	30	31	22	20	21	12	10	11	02	00	01
22	31	32	30	21	22	20	11	12	10	01	02	00
30	10	11	12	00	01	02	30	31	32	20	21	22
31	12	10	11	02	00	01	32	30	31	22	20	21
32	11	12	10	01	02	00	31	32	30	21	22	20

Fig. 3 A pair of orthogonal Latin squares of order 12

Proof We begin by verifying that there exists an arrangement of the rows of both arrays $A_1 \otimes A_2$ and $B_1 \otimes B_2$, which verifies that they are quasi-Sudoku Latin squares.

For fixed q, the entries $A_1(p, q)$ and $B_1(p, q)$ take the values in column q of A_1 and B_1, respectively. That is, for fixed q, $\{A_1(p, q) \mid 0 \le p \le m-1\} = \{B_1(p, q) \mid 0 \le p \le m-1\} = [m]$. Likewise, for fixed s, the entries $A_2(s, t)$ and $B_2(s, t)$ take values in row s of A_2 and B_2, respectively. That is, for fixed s, $\{A_2(s, t) \mid 0 \le t \le n-1\} = \{B_2(s, t) \mid 0 \le t \le n-1\} = [n]$. Thus, for fixed q and s

$$\begin{aligned} [m] \times [n] &= \{(A_1(p, q), A_2(s, t)) \mid 0 \le p \le m-1, 0 \le t \le n-1\} \\ &= \{(B_1(p, q), B_2(s, t)) \mid 0 \le p \le m-1, 0 \le t \le n-1\}. \end{aligned}$$

Hence, we will assume that the rows of $A_1 \otimes A_2$ and $B_1 \otimes B_2$ have been reordered by moving row $np + s$ to position $ms + p$, where $0 \le p \le m-1$ and $0 \le s \le n-1$. The order of the columns, however, remains as $qn + t$, where $0 \le q \le m-1$ and $0 \le t \le n-1$. Now for fixed s and q, the subarrays of $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are defined by the intersection of rows $ms + p$ with columns $qn + t$, where $0 \le p \le m - 1$ and $0 \le t \le n - 1$ contain each of the mn entries precisely once. Note that the reordering of rows has been consistently applied to both $A_1 \otimes A_2$ and $B_1 \otimes B_2$; therefore these Latin squares are still orthogonal.

For the remainder of the proof, we will replace q by $\overline{q}$ and s by $\overline{s}$ to emphasize the fact that these two parameters are fixed. In addition, in the reordered squares, fixed $\overline{q}$ and $\overline{s}$ define a subarray containing all entries of $[m] \times [n]$.

We select two onto functions $\Pi_m : [m] \times [n] \to [m]$ and $\Pi_n : [m] \times [n] \to [n]$, such that if $\Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t)) = \Pi_m(A_1(p', \overline{q}), A_2(\overline{s}, t'))$, then $t \neq t'$, and if $\Pi_n(B_1(p, \overline{q}), B_2(\overline{s}, t)) = \Pi_n(B_1(p', \overline{q}), B_2(\overline{s}, t'))$, then $t = t'$. The first projection ensures that in the subarray of $A_1 \otimes A_2$ (defined by $\overline{q}$ and $\overline{s}$) in each column, the entries are distinct and the second projection ensures that in this subarray and in each column the entries are all the same.

Such functions are not hard to find; for instance, we could take

$$\Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t)) = A_1(p, \overline{q}) \text{ and}$$
$$\Pi_n(B_1(p, \overline{q}), B_2(\overline{s}, t)) = B_2(\overline{s}, t),$$

or if m and n are coprime, with $m > n$, take

$$\Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t)) = (n \times A_1(p, \overline{q}) + A_2(\overline{s}, t)) \bmod m \text{ and}$$
$$\Pi_n(B_1(p, \overline{q}), B_2(\overline{s}, t)) = (n \times B_1(p, \overline{q}) + B_2(\overline{s}, t)) \bmod n.$$

In this latter case, since m and n are coprime and $m > n$, for fixed $\overline{q}$, $\{n \times A_1(p, \overline{q}) \bmod m \mid 0 \le p \le m - 1\} = [m]$ and for a fixed column t, so fixed $A_2(\overline{s}, t)$, $\{n \times A_1(p, \overline{q}) + A_2(\overline{s}, t) \bmod m \mid 0 \le p \le m - 1\} = [m]$. Further, $n \times B_1(p, \overline{q}) + B_2(\overline{s}, t) \equiv B_2(\overline{s}, t) \bmod n$, so $\{\Pi_n((B_1(p, \overline{q}), B_2(\overline{s}, t))) \mid 0 \le p \le m - 1, 0 \le t \le n\} = [n]$. Thus, $\{(\Pi_m((A_1(p, \overline{q}), A_2(\overline{s}, t))), \Pi_n((B_1(p, \overline{q}), B_2(\overline{s}, t))) \mid 0 \le p \le m - 1, 0 \le t \le n\} = [m] \times [n]$. This verifies that $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are doubly orthogonal quasi-Sudoku squares. □

It should be noted that the different projections given in the above proof produce non-isomorphic squares. This will be illustrated in the example given below. For $m = n$, the extension of these pairwise properties to more than two orthogonal direct product designs is immediate, if the component designs are available. Further, it should be noted that when we have that $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are orthogonal quasi-Sudoku Latin squares, we are assuming that the rows of the direct products have been rearranged to the required format for Sudoku Latin squares.

4 An example

As an illustration, we will construct doubly orthogonal quasi-Sudoku Latin squares of order 12. We begin with two orthogonal Latin squares of order $n = 3$ and two of the three orthogonal Latin squares of order $m = 4$, as shown in Fig. 2. Note, it does not matter which two orthogonal Latin squares of order 4 we choose, so we

Reordered $A_1 \otimes A_2$

	00	01	02	10	11	12	20	21	22	30	31	32
00	00	01	02	10	11	12	20	21	22	30	31	32
10	10	11	12	00	01	02	30	31	32	20	21	22
20	20	21	22	30	31	32	00	01	02	10	11	12
30	30	31	32	20	21	22	10	11	12	00	01	02
01	01	02	00	11	12	10	21	22	20	31	32	30
11	11	12	10	01	02	00	31	32	30	21	22	20
21	21	22	20	31	32	30	01	02	00	11	12	10
31	31	32	30	21	22	20	11	12	10	01	02	00
02	02	00	01	12	10	11	22	20	21	32	30	31
12	12	10	11	02	00	01	32	30	31	22	20	21
22	22	20	21	32	30	31	02	00	01	12	10	11
32	32	30	31	22	20	21	12	10	11	02	00	01

Reordered $B_1 \otimes B_2$

	00	01	02	10	11	12	20	21	22	30	31	32
00	00	01	02	10	11	12	20	21	22	30	31	32
10	20	21	22	30	31	32	00	01	02	10	11	12
20	30	31	32	20	21	22	10	11	12	00	01	02
30	10	11	12	00	01	02	30	31	32	20	21	22
01	02	00	01	12	10	11	22	20	21	32	30	31
11	22	20	21	32	30	31	02	00	01	12	10	11
21	32	30	31	22	20	21	12	10	11	02	00	01
31	12	10	11	02	00	01	32	30	31	22	20	21
02	01	02	00	11	12	10	21	22	20	31	32	30
12	21	22	20	31	32	30	01	02	00	11	12	10
22	31	32	30	21	22	20	11	12	10	01	02	00
32	11	12	10	01	02	00	31	32	30	21	22	20

Fig. 4 A pair of orthogonal quasi-Sudoku Latin squares of order 12

arbitrarily select the first and the last. In general, if the underlying Latin squares are non-isomorphic, then it is possible to construct sets of non-isomorphic doubly orthogonal quasi-Sudoku Latin squares.

In Fig. 3, we construct $A_1 \otimes A_2$ and $B_1 \otimes B_2$ using the direct product construction. To facilitate understanding, rows and columns have been labelled and (x, y) has been replaced by xy. In Fig. 4, the rows have been reordered as first $(p, 0)$ for $0 \leq p \leq 3$, then $(p, 1)$ for $0 \leq p \leq 3$, then $(p, 2)$ for $0 \leq p \leq 3$ to emphasise the fact that these squares are quasi-Sudoku Latin squares.

In Fig. 5, we project down each subsquare in Fig. 4 by applying the mappings $\Pi_4 : [4] \times [3] \to [4]$ and $\Pi_3 : [4] \times [3] \to [3]$, given by

$$\Pi_4((A_1(p,q), A_2(s,t))) = (3 \times A_1(p,q) + A_2(s,t)) \bmod 4, \text{ and}$$
$$\Pi_3((B_1(p,q), B_2(s,t))) = (3 \times B_1(p,q) + B_2(s,t)) \bmod 3,$$

to the entries in the quasi-Sudoku squares obtained by reordering the rows of the Latin squares $A_1 \otimes A_2$ and $B_1 \otimes B_2$ and label these as $\Pi_4(A_1 \otimes A_2)$ and $\Pi_3(B_1 \otimes B_2)$. Then,

$\Pi_4(A_1 \otimes A_2)$

	00	01	02	10	11	12	20	21	22	30	31	32
00	0	1	2	3	0	1	2	3	0	1	2	3
10	3	0	1	0	1	2	1	2	3	2	3	0
20	2	3	0	1	2	3	0	1	2	3	0	1
30	1	2	3	2	3	0	3	0	1	0	1	2
01	1	2	0	0	1	3	3	0	2	2	3	1
11	0	1	3	1	2	0	2	3	1	3	0	2
21	3	0	2	2	3	1	1	2	0	0	1	3
31	2	3	1	3	0	2	0	1	3	1	2	0
02	2	0	1	1	3	0	0	2	3	3	1	2
12	1	3	0	2	0	1	3	1	2	0	2	3
22	0	2	3	3	1	2	2	0	1	1	3	0
32	3	1	2	0	2	3	1	3	0	2	0	1

$\Pi_3(B_1 \otimes B_2)$

	00	01	02	10	11	12	20	21	22	30	31	32
00	0	1	2	0	1	2	0	1	2	0	1	2
10	0	1	2	0	1	2	0	1	2	0	1	2
20	0	1	2	0	1	2	0	1	2	0	1	2
30	0	1	2	0	1	2	0	1	2	0	1	2
01	2	0	1	2	0	1	2	0	1	2	0	1
11	2	0	1	2	0	1	2	0	1	2	0	1
21	2	0	1	2	0	1	2	0	1	2	0	1
31	2	0	1	2	0	1	2	0	1	2	0	1
02	1	2	0	1	2	0	1	2	0	1	2	0
12	1	2	0	1	2	0	1	2	0	1	2	0
22	1	2	0	1	2	0	1	2	0	1	2	0
32	1	2	0	1	2	0	1	2	0	1	2	0

Fig. 5 Orthogonal quasi-Sudoku Latin squares under projections Π_4 and Π_3

in Fig. 6, we superimpose the projections $\Pi_4(A_1 \otimes A_2)$ and $\Pi_3(B_1 \otimes B_2)$ to verify that indeed $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are doubly orthogonal quasi-Sudoku Latin squares of order 12, as each 4×3 subsquare has each of the ordered pairs (x, y), $0 \leq x \leq 3$ and $0 \leq y \leq 2$.

If the projections Π_4 and Π_3, given above, are replaced by the projections

$$\begin{aligned} \Pi_4((A_1(p,q), A_2(s,t))) &= A_1(p,q), \text{ and} \\ \Pi_3((B_1(p,q), B_2(s,t))) &= B_2(s,t), \end{aligned}$$

we obtain the projected squares given in Fig. 7. Note that here each of the twelve subsquares can be obtained by reordering the rows and/or the columns of the first subsquare. This is not the case for the projected squares given in Fig. 6. To see this, consider the first subsquare and any of the subsquares on rows 01, 11, 21 and 31 of Fig. 6; setwise the rows of these subsquares do not equal any row in the first subsquare.

$\Pi_4(A_1 \otimes A_2), \Pi_3(B_1 \otimes B_2)$

	00	01	02	10	11	12	20	21	22	30	31	32
00	0,0	1,1	2,2	3,0	0,1	1,2	2,0	3,1	0,2	1,0	2,1	3,2
10	3,0	0,1	1,2	0,0	1,1	2,2	1,0	2,1	3,2	2,0	3,1	0,2
20	2,0	3,1	0,2	1,0	2,1	3,2	0,0	1,1	2,2	3,0	0,1	1,2
30	1,0	2,1	3,2	2,0	3,1	0,2	3,0	0,1	1,2	0,0	1,1	2,2
01	1,2	2,0	0,1	0,2	1,0	3,1	3,2	0,0	2,1	2,2	3,0	1,1
11	0,2	1,0	3,1	1,2	2,0	0,1	2,2	3,0	1,1	3,2	0,0	2,1
21	3,2	0,0	2,1	2,2	3,0	1,1	1,2	2,0	0,1	0,2	1,0	3,1
31	2,2	3,0	1,1	3,2	0,0	2,1	0,2	1,0	3,1	1,2	2,0	0,1
02	2,1	0,2	1,0	1,1	3,2	0,0	0,1	2,2	3,0	3,1	1,2	2,0
12	1,1	3,2	0,0	2,1	0,2	1,0	3,1	1,2	2,0	0,1	2,2	3,0
22	0,1	2,2	3,0	3,1	1,2	2,0	2,1	0,2	1,0	1,1	3,2	0,0
32	3,1	1,2	2,0	0,1	2,2	3,0	1,1	3,2	0,0	2,1	0,2	1,0

Fig. 6 The projected squares verifying that $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are doubly orthogonal quasi-Sudoku Latin squares of order 12

$\Pi_4(A_1 \otimes A_2), \Pi_3(B_1 \otimes B_2)$

	00	01	02	10	11	12	20	21	22	30	31	32
00	0,0	0,1	0,2	1,0	1,1	1,2	2,0	2,1	2,2	3,0	3,1	3,2
10	1,0	1,1	1,2	0,0	0,1	0,2	3,0	3,1	3,2	2,0	2,1	2,2
20	2,0	2,1	2,2	3,0	3,1	3,2	0,0	0,1	0,2	1,0	1,1	1,2
30	3,0	3,1	3,2	2,0	2,1	2,2	1,0	1,1	1,2	0,0	0,1	0,2
01	0,2	0,0	0,1	1,2	1,0	1,1	2,2	2,0	2,1	3,2	3,0	3,1
11	1,2	1,0	1,1	0,2	0,0	0,1	3,2	3,0	3,1	2,2	2,0	2,1
21	2,2	2,0	2,1	3,2	3,0	3,1	0,2	0,0	0,1	1,2	1,0	1,1
31	3,2	3,0	3,1	2,2	2,0	2,1	1,2	1,0	1,1	0,2	0,0	0,1
02	0,1	0,2	0,0	1,1	1,2	1,0	2,1	2,2	2,0	3,1	3,2	3,0
12	1,1	1,2	1,0	0,1	0,2	0,0	3,1	3,2	3,0	2,1	2,2	2,0
22	2,1	2,2	2,0	3,1	3,2	3,0	0,1	0,2	0,0	1,1	1,2	1,0
32	3,1	3,2	3,0	2,1	2,2	2,0	1,1	1,2	1,0	0,1	0,2	0,0

Fig. 7 The projected squares verifying that $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are doubly orthogonal quasi-Sudoku Latin squares of order 12

5 Quasi-sliced orthogonal arrays

A (symmetric) orthogonal array, denoted $OA(N, k, s, t)$, is an $N \times k$ array with entries chosen from the set $[s]$ of levels, such that for every $N \times t$ submatrix the s^t level combinations of $\overbrace{[s] \times \cdots \times [s]}^{t}$ each occur a constant number of times. We follow the work of Qian and Wu (2009) and define a sliced symmetric orthogonal array to be an $OA(N, k, s, t)$, $\mathcal{O}$, which satisfies the following property:

- there exists a projection Π from $[s]$ to $[s_0]$, $s_0 < s$, and a partition of the rows of $\mathcal{O}$ into ν subarrays, $\mathcal{O}_i$, such that when the s levels of $[s]$ are collapsed according to the projection Π each $\mathcal{O}_i$ forms a symmetric $OA(N_0, k, s_0, t)$.

We say $(\mathcal{O}_1, \mathcal{O}_2, \ldots, \mathcal{O}_\nu)$ is a sliced symmetric orthogonal array.

For a k factor design, let $S = (s_1, \ldots, s_k)$ denote the list of numbers of factor levels. An asymmetric orthogonal array, denoted $OA(N, k, S, t)$, is an $N \times k$ array, where the jth column contains entries of $[s_j]$, $s_j \in S$, and for each t-subset T of columns, the $N \times t$ submatrix defined by these columns contains all $\prod_{i \in T} s_i$ tuples of $\prod_{i \in T}[s_i]$ (the Cartesian product of $[s_i]$, $i \in T$) a constant, λ_T, number of times. We define a quasi-sliced asymmetric orthogonal array to be an $OA(N, k, S, t)$ array, $\mathcal{O}$, which satisfies the following property:

- there exist projections $\Pi_i : [s_i] \to [s_i']$ for $i = 1, \ldots, k$ and a partition of the rows $\mathcal{O}$ into ν subarrays, $\mathcal{O}_i$, such that when the sets of levels $[s_1], \ldots, [s_k]$ are respectively collapsed onto $[s_1'], \ldots, [s_k']$, $s_i' < s_i$, each $\mathcal{O}_i$ is an asymmetric $OA(N_0, k, S', t)$, $S' = (s_1', s_2', \ldots, s_k')$.

More precisely, $(\mathcal{O}_1, \ldots, \mathcal{O}_\nu)$ is said to be a quasi-sliced asymmetric orthogonal array. We note that if the projection Π_i is not one-to-one, then it is immediate that $s_i' < s_i$. Also if $S = \{s\}$ and the orthogonal array is symmetric, we revert to the notation $OA(N, k, s, t)$.

Li et al. (2015) give four constructions for balanced sliced asymmetric orthogonal arrays based on similar "producting" techniques. Here, the term balanced implies the orthogonal arrays satisfy strength one conditions. The first three constructions given in Li et al. (2015) use difference matrices (Hedayat et al. 2012) as a basic ingredient. It is well known that difference matrices can be used to construct $OA(N, k, s, 2)$ orthogonal arrays and hence mutually orthogonal Latin squares. However, very little is known about difference matrices except those constructed from finite fields and hence of prime power order. By contrast, the construction presented in the current paper only assumes the existence of pairs of orthogonal Latin squares, which are known to exist for all orders except 2 and 6 with a broader range of techniques. The details of alternate construction techniques can be found in Colbourn and Dinitz (2006). In addition, the projections used by Li et al. (2015) must satisfy the additive property; that is, $\Pi(f + g) = \Pi(f) + \Pi(g)$. Here, it is required that the functions Π_m and Π_n are onto. The final construction given by Li, Jiang and Ai assumes the existence of a pair of symmetric balanced sliced orthogonal arrays A, $OA(n_1, m_1, s_1, 2)$ and B, $OA(s_1, m_2, r_1, 2)$ and projections δ_1 and δ_2 that, respectively, result in orthogonal arrays $OA(n_2, m_1, s_2, 2)$ and $OA(s_2, m_2, r_2, 2)$. Thus, the number of runs in B is equal to the number of levels in A. This condition places some restrictions on the application of such constructions. Ai et al. (2014) used similar techniques to construct symmetric balanced sliced orthogonal arrays. In these constructions, it was assumed that for each factor the levels were partitioned into subclasses of the same size and that any two elements in the same partition were projected onto the same element, an assumption that implies that the resulting space-filling designs achieve maximum stratification in the univariate margins as well as stratification in the higher-dimensional margins. If in the proof of Proposition 2 we assume that for the function Π_m and Π_n each point in the range is the image of, respectively, n and m points in the domain, then the constructions here achieve maximum stratification in the univariate margins and stratification of the bivariate margins. Once again, there are many distinct functions that satisfy this property. As stated earlier, the main advantage of the results presented here is that the construction is relatively well described and straightforward, and consequently easy to implement and available for a broad range of sizes (Colbourn and Dinitz 2006; Keedwell and Dénes 2015; Raghavarao 1971).

Proposition 3 *If A_1 and B_1 are pairwise orthogonal Latin squares of order m, and A_2 and B_2 are pairwise orthogonal Latin squares of order n, then there exists an orthogonal array $OA(m^2n^2, 4, mn, 2)$, which satisfies the properties of a quasi-sliced asymmetric orthogonal array, in that after collapsing each slice is an $OA(mn^2, 4, S', 2)$, where $S' = (n, n, m, n)$.*

Proof "Unstack" the pair of orthogonal quasi-Sudoku Latin squares $A_1 \otimes A_2$ and $B_1 \otimes B_2$ to obtain an orthogonal array $OA(m^2n^2, 4, mn, 2)$, $\mathcal{O}$, where row (r, c) of $\mathcal{O}$ takes the form

$$\big[\, r,\ c,\ (A_1 \otimes A_2)(r, c),\ (B_1 \otimes B_2)(r, c) \,\big].$$

To verify that this is a quasi-sliced asymmetric orthogonal array, we provide details of the partitioning of the rows of OA and then verify that there exists projections such that each partition corresponds to an $OA(m^2n^2, 4, S', 2)$, where $S' = (n, n, m, n)$.

Recall that the rows of the reordered squares $A_1 \otimes A_2$ and $B_1 \otimes B_2$ are labelled as (p, s), $0 \leq p \leq m-1$ and $0 \leq s \leq n-1$, and the columns are labelled as (q, t), $0 \leq q \leq m-1$ and $0 \leq t \leq n-1$. Now for fixed $q = \overline{q}$, let $\mathcal{O}_{\overline{q}}$ be the $(mn^2) \times 4$ subarray with rows indexed by $((p, s), (\overline{q}, t))$, $0 \leq p \leq m-1$ and $0 \leq s, t \leq n-1$, so each row of $\mathcal{O}_{\overline{q}}$ is of the form

$$\big[\, \Pi_1(p, s),\ \Pi_2(\overline{q}, t),\ \Pi_m(A_1 \otimes A_2)((p, s), (\overline{q}, t)),\ \Pi_n(B_1 \otimes B_2)((p, s), (\overline{q}, t)) \,\big],$$

where $\Pi_1 : (p, s) \rightarrow s$, $\Pi_2 : (\overline{q}, t) \rightarrow t$ and Π_m and Π_n are defined in the proof of Proposition 2. Note that each of these projections is not one to one.

Now, we need to prove that $\mathcal{O}_{\overline{q}}$ is an asymmetric orthogonal array with parameters $OA(mn^2, 4, S', 2)$ where $S' = (n, n, m, n)$.

Note that for fixed $s = \overline{s}$ columns 3 and 4 of $\mathcal{O}_{\overline{q}}$, are the concatenation of the n sets of pairs

$$\Big\{\Big(\Pi_m\big(A_1(p, \overline{q}), A_2(\overline{s}, t)\big), \Pi_n\big(B_1(p, \overline{q}), B_2(\overline{s}, t)\big)\Big) \\ \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\Big\} = [m] \times [n]$$

one set for each of the $m \times n$ subarrays in the Latin squares. Hence, columns 3 and 4 are the concatenation of n copies of $[m] \times [n]$.

Next, recall that in the proof of Proposition 2, the projections Π_m and Π_n were chosen to ensure that in the $m \times n$ subarray of the Latin square $A_1 \otimes A_2$, the entries in each column are distinct, and in $B_1 \otimes B_2$ the entries in each column are all the same but the entries in the rows are distinct.

For fixed $s = \overline{s}$, the set of pairs $\{(\Pi_1(p, \overline{s}), \Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\} = \{(\overline{s}, \Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq$

$t \leq n-1\}$ gives n copies of $\{\overline{s}\} \times [m]$, one for each column of the subarray. Further, $\{(\Pi_1(p, \overline{s}), (\Pi_n(B_1(p, \overline{q}), B_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\} = \{(\overline{s}, (\Pi_n(B_1(p, \overline{q}), B_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\}$ giving m copies of $\{\overline{s}\} \times [n]$. So, respectively, as s takes the values $0, \ldots, n-1$, we obtain n copies of $[n] \times [m]$ and m copies of $[n] \times [n]$.

For fixed $s = \overline{s}$, the set of pairs $\{(\Pi_2((\overline{q}, t), \Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\} = \{(t, \Pi_m(A_1(p, \overline{q}), A_2(\overline{s}, t))) \mid 0 \leq p \leq m-1, 0 \leq t \leq n-1\}$ gives one copy of $[n] \times [m]$. So, as s takes the values $0, \ldots, n-1$, we obtain n copies of $[n] \times [m]$. Finally for fixed $p = \overline{p}$, $\{(\Pi_2(\overline{q}, t), \Pi_n(B_1(\overline{p}, \overline{q}), B_2(s, t))) \mid 0 \leq s, t \leq n-1\} = \{(t, \Pi_n(B_1(\overline{p}, \overline{q}), B_2(s, t))) \mid 0 \leq st \leq n-1\}$ gives 1 copy of $[n] \times [n]$, and as for $0 \leq p \leq m-1$, m copies of $[n] \times [n]$.

Thus each $\mathcal{O}_q$ for $0 \leq q \leq m-1$ is an asymmetric orthogonal array with the required parameters. In all cases, the projections are not one-to-one and the result is a quasi-sliced asymmetric orthogonal array as required. □

By way of example, we project the first three columns of the array given in Fig. 6 to obtain the slice of the orthogonal array, denoted $\mathcal{O}_0$ ($q = 0$) with parameters $OA(36, 4, S', 2)$, where $S' = (3, 3, 4, 3)$. The transpose of this slice is given below. Note that the projection Π_1 has been applied to the rows' labels in Fig. 6, giving the values in the first row of the following array, and Π_2 has been applied to the column labels in Fig. 6, giving the values in the second row of the following array.

In principle, it is possible to construct quasi-sliced orthogonal arrays for $k > 4$; however, the construction relies on first constructing the doubly orthogonal quasi-Sudoku Latin squares. When $n = m = p$, such an approach could be possible, but onerous to verify and to implement for $k > 4$. In addition, it might be possible to achieve a construction where all factors, with the exception of one factor, had the same number of levels, but once again very onerous to implement. In these cases, it may be better to revert to Tang's construction (Tang 1993) or adapt the algorithm given in Donovan et al. (2015).

6 Construction of quasi-Sudoku-based sliced space-filling designs

Sliced space-filling designs can be constructed from the doubly orthogonal quasi-Sudoku Latin squares or the quasi-sliced asymmetric orthogonal arrays using the techniques in Qian and Wu (2009), Tang (1993) and Xu et al. (2011). In brief, the procedure follows the steps given below.

- S1 Use the direct product construction as specified in Sect. 3 to construct orthogonal Latin squares of composite order mn from orthogonal Latins squares of order m and n.
- S2 Rearrange the rows of these squares to obtain orthogonal quasi-Sudoku Latin squares of order mn.
- S3 Identify projection Π_m and Π_n and use these to verify the existence of doubly orthogonal quasi-Sudoku Latin squares of order mn.
- S4 "Unstack" the Latin squares to obtain a quasi-sliced $OA(m^2n^2, 4, mn, 2)$, where each partition can be collapsed to a slice corresponding to an $OA(m^2n^2, 4, S', 2)$, where $S' = (n, n, m, n)$.

$\mathcal{O}_0$ after projections Π_1 and Π_2 have been applied.

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

Fig. 8 The projected sliced array $\mathcal{O}_0'$

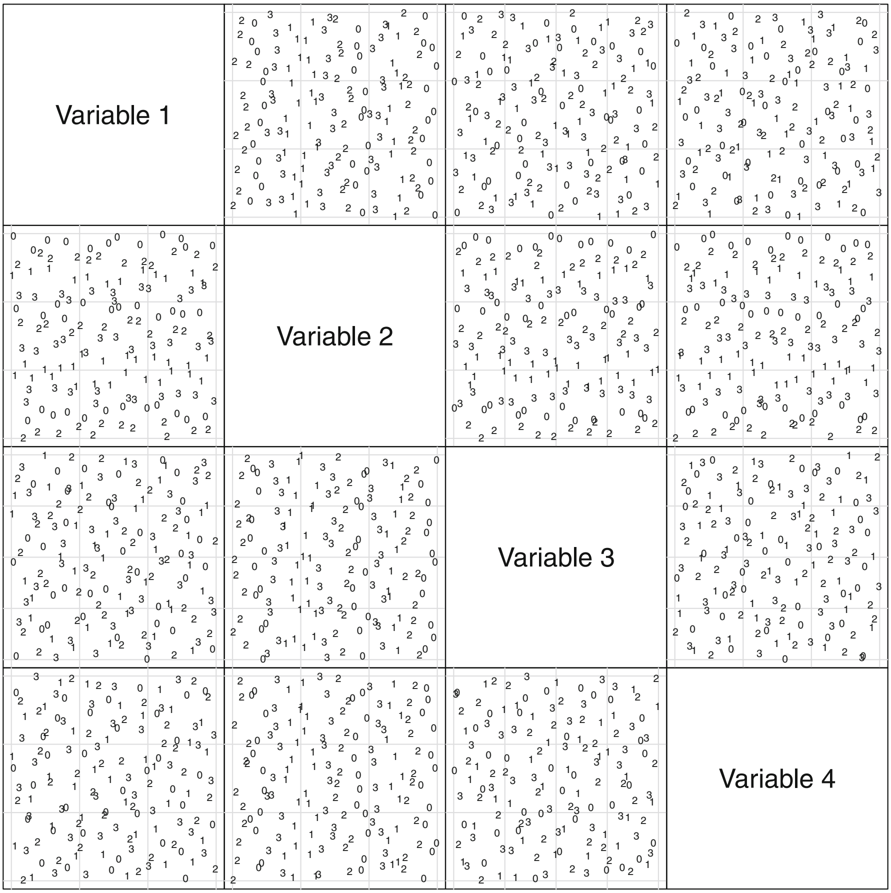

Fig. 9 Sliced space-filling design based on a quasi-sliced asymmetric orthogonal array. Slices are indicated by point labels

S5 Group the runs of each slice together.

S6 Randomly relabel the element of each column of each slice using the labels $1, \ldots, mn$ and subject to the constraint that the elements mapped to the same symbol by Π form a consecutive subset of $1, \ldots, mn$.

S7 For each column replace each symbol k with a random permutation of $(k-1)mn+1, \ldots, (k-1)mn+mn$.

S8 Construct a space-filling design with points generated as $(x_{ij} - u_{ij})/(mn)^2$, where x_{ij} denotes the design elements after step S7 and u_{ij} denotes a random Uniform$(0, 1)$ deviate.

As an example, Fig. 9 shows a sliced space-filling design constructed based on the quasi-sliced asymmetric orthogonal array whose first slice is shown in Fig. 8.

As shown in Qian and Wu (2009) and Xu et al. (2011), the complete design achieves uniformity in one- and two-dimensional projections, while the slices are guaranteed to achieve uniformity in two-dimensional projections. On the other hand, the columns based on the doubly orthogonal quasi-Sudoku Latin squares can be divided into a larger number of slices, as defined by the quasi-Sudoku sub-squares, each of which has guaranteed uniformity under one- and two-dimensional projections, as shown in Xu et al. (2011).

References

Ai, M., Jiang, B., Li, K. (2014). Construction of sliced space-filling designs based on balanced sliced orthogonal arrays. *Statistica Sinica*, *24*, 1685–1702.

Colbourn, C. J., Dinitz, J. H. (2006). *Handbook of combinatorial designs*. New York: CRC Press.

Donovan, D., Burrage, K., Burrage, P., McCourt, T. A., Thompson, H. B., Yazici, E. S. (2015). Estimates of the coverage of parameter space by latin hypercube and orthogonal sampling: connections between populations of models and experimental designs. Preprint arXiv:1510.03502.

Haaland, B., Qian, P. Z. (2010). An approach to constructing nested space-filling designs for multi-fidelity computer experiments. *Statistica Sinica*, *20*(3), 1063.

Hedayat, A. S., Sloane, N. J. A., Stufken, J. (2012). *Orthogonal arrays: theory and applications*. New York: Springer Science & Business Media.

Keedwell, A. D., Dénes, J. (2015). *Latin squares and their applications*. New York: Elsevier.

Li, K., Jiang, B., Ai, M. (2015). Sliced space-filling designs with different levels of two-dimensional uniformity. *Journal of Statistical Planning and Inference*, *157*, 90–99.

Pedersen, R. M., Vis, T. L. (2009). Sets of mutually orthogonal sudoku latin squares. *The College Mathematics Journal*, *40*(3), 174–181.

Qian, P. Z., Wu, C. J. (2009). Sliced space-filling designs. *Biometrika*, *96*(4), 945–956.

Raghavarao, D. (1971). *Constructions and combinatorial problems in design of experiments* (Vol. 4). New York: Wiley.

Tang, B. (1993). Orthogonal array-based latin hypercubes. *Journal of the American statistical association*, *88*(424), 1392–1397.

USA Today. (2013). Daily crossword. 19 September 2013.

Xu, X., Haaland, B., Qian, P. Z. (2011). Sudoku-based space-filling designs. *Biometrika*, *98*(3), 711–720.

Zhang, Q., Qian, P. Z. (2013). Designs for crossvalidating approximation models. *Biometrika*, *100*(4), 997–1004.