Journal of the American Statistical Association

ISSN: (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/uasa20

A Method of Constructing Space-Filling Orthogonal Designs

Fasheng Sun & Boxin Tang

To cite this article: Fasheng Sun & Boxin Tang (2017) A Method of Constructing Space-Filling Orthogonal Designs, Journal of the American Statistical Association, 112:518, 683-689, DOI: 10.1080/01621459.2016.1159211

To link to this article: https://doi.org/10.1080/01621459.2016.1159211

Published online: 30 Mar 2017.

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION
2017, VOL. 112, NO. 518, 683–689, Theory and Methods
https://doi.org/10.1080/01621459.2016.1159211

A Method of Constructing Space-Filling Orthogonal Designs

Fasheng Sun[a] and Boxin Tang[b]

[a]Key Laboratory for Applied Statistics of MOE and School of Mathematics and Statistics, Northeast Normal University, Changchun, China; [b]Department of Statistics and Actuarial Science, Simon Fraser University, Burnaby, British Columbia, Canada

ABSTRACT
This article presents a method of constructing a rich class of orthogonal designs that include orthogonal Latin hypercubes as special cases. Two prominent features of the method are its simplicity and generality. In addition to orthogonality, the resulting designs enjoy some attractive space-filling properties, making them very suitable for computer experiments.

ARTICLE HISTORY
Received July 2015
Revised December 2015

KEYWORDS
Computer experiment; Expansive replacement method; Latin hypercube; Level collapsing; Orthogonal array; Rotation-in-groups

1. Introduction

The study of orthogonal Latin hypercubes has been of considerable interest in the literature of designing computer experiments. Although some research had been done earlier on nearly orthogonal Latin hypercubes, Ye (1998) was the first to construct Latin hypercubes that are exactly orthogonal. This line of research was further pursued, resulting significant enhancements in the methods and results, in Steinberg and Lin (2006), Lin, Mukerjee, and Tang (2009), Pang, Liu and Lin (2009), Sun, Liu, and Lin (2009), and Lin et al. (2010). It was argued in Bingham, Sitter, and Tang (2009) that orthogonal designs with many levels are as suitable for computer experiments as orthogonal Latin hypercubes. Construction of such orthogonal designs was further studied by Georgiou (2011). Orthogonality is of importance when polynomial modeling is considered, and can also be viewed as a simple device to get closer to space-filling designs.

It has been widely accepted that space-filling designs are appropriate for computer experiments especially when Gaussian process models are under consideration (Santner, Williams, and Notz 2003; Fang, Li, and Sudjianto 2006). One approach of constructing space-filling designs is through computer search using popular criteria based on measures of discrepancy or distance; an example of such work is that of Joseph and Hung (2008) who considered the construction of orthogonal-maximin Latin hypercube designs. A more fruitful approach is to construct designs that are space-filling in low-dimensional projections using orthogonal arrays or similar structures. This went back to McKay, Beckman, and Conover (1979) who introduced Latin hypercubes, which are orthogonal arrays of strength one. Owen (1992) and Tang (1993) considered randomized orthogonal arrays and orthogonal array-based Latin hypercubes, representing an important development in this area. More recently, He and Tang (2013) introduced strong orthogonal arrays and Mukerjee, Sun, and Tang (2014) studied mappable nearly orthogonal arrays, both with the purpose of constructing better space-filling designs than those based on ordinary orthogonal arrays.

This article presents a general method of constructing orthogonal designs that are space-filling in low-dimensional projections. Though the basic idea of rotation-in-groups as in Steinberg and Lin (2006), Lin, Mukerjee, and Tang (2009), and Pang, Liu, and Lin (2009) is still relevant, our new method enjoys several advantages. It is simple, requiring no use of finite fields and projective geometries. Our method is general, not only in the flexibility of the run size and the number of levels but also in the capability of constructing a broader class of orthogonal designs than orthogonal Latin hypercubes. Most importantly, the method produces designs that are not just orthogonal but also space-filling in low dimensions—this, in fact, is the primary motivation behind the work in this article.

We conclude this section with a general discussion on the modeling and analysis of computer experiments. Gaussian process models are commonly employed for analyzing data from computer experiments (Santner, Williams, and Notz 2003). It has been widely accepted that space-filling designs are appropriate for such models. One formal justification for space-filling designs was given in Johnson, Moore, and Ylvisaker (1990) who showed that minimax and maximin distance designs are asymptotically optimal when the correlations are getting weak. Another justification for space-filling designs is their robustness to model misspecification, the idea of which went back to Box and Draper (1959) and Sacks and Ylvisaker (1984) who showed that spreading the design points uniformly in the design region has an effect of minimizing the bias of the fitted model. In an exploratory investigation where the experimenter aims at identifying a few dominant factors out of a large number of factors—the screening experiment setting, polynomial models with the first and perhaps also second-order terms are very convenient to use (Ye 1998). Such models should be well served by orthogonal Latin hypercube designs or more generally orthogonal designs

CONTACT Boxin Tang boxint@sfu.ca Department of Statistics and Actuarial Science, Simon Fraser University Burnaby, British Columbia V5A 1S6, Canada.

with many levels. Our work in this article constructs a class of designs that are not just orthogonal but also space-filling, which should therefore be very suitable for computer experiments as one now has the flexibility of contemplating the use of both Gaussian process models and polynomial models. This provides a kind of robust property that has a flavor similar to the estimation capacity for fractional factorial designs discussed in Cheng, Steinberg, and Sun (1999).

2. Method and Results

2.1. Notation and Preliminaries

We use $D(n, s^m)$ to denote a balanced design of n runs for m factors, with each of the s levels replicated equally often. When $s = n$, design $D(n, s^m)$ becomes a Latin hypercube. To facilitate the study of orthogonality, the s levels are equally spaced, centered, and taken to be

$$\Omega(s) = \{u - (s+1)/2 \mid u = 1, \ldots, s\}, \quad (1)$$

where the uth level is given by $u - (s+1)/2$ for $u = 1, \ldots, s$. Thus, the levels are $-0.5, 0.5$ for $s = 2$ and $-1, 0, 1$ for $s = 3$. A $D(n, s^m)$ is said to be orthogonal if $d_i^T d_j = 0$ for any two of its columns d_i and d_j; in this case, we use $OD(n, s^m)$ to denote such an orthogonal design. A $D(n, s^m)$ becomes an orthogonal array of strength t if each t-tuple occurs the same number of times in any of its $n \times t$ submatrix; such an orthogonal array is denoted by $OA(n, s^m, t)$. For an $OA(n, s^m, t)$, we must have $n = \lambda s^t$ for some integer λ, which is called the index of the array. Obviously, any $D(n, s^m)$ is an orthogonal array of strength one and any $OA(n, s^m, t)$ with $t \geq 2$ is an $OD(n, s^m)$.

Let A be an $OA(n, s^{m_1}, 2)$ and B an $OA(s, p^{m_2}, 2)$, where s and p need not be prime powers, though they often are. In each column of A, if we replace the uth level, for $u = 1, \ldots, s$, by the uth row of B, then the resulting matrix C must be an $OA(n, p^{m_1 m_2}, 2)$. This is the expansive replacement method discussed in Hedayat, Sloane, and Stufken (1999, sec. 9.3). Crucial to our article is another property of the resulting array C, an $OA(n, p^{m_1 m_2}, 2)$, which we discuss next. Though simple, this property has not been mentioned in the literature, at least to the best of our knowledge. To be precise and also for the later development, write C as

$$C = (C_1, C_2, \ldots, C_{m_1}), \quad (2)$$

where C_i represents the ith group of m_2 columns arising from replacing the levels in the ith column of A by the rows of B. Then we have the following result.

Proposition 1. Any four columns, obtained by taking two columns from one group C_{i_1} and two columns from another group C_{i_2} where $i_1 \neq i_2$ must form an $OA(n, p^4, 4)$, a strength four array.

The result is quite intuitive. We provide a proof nonetheless in the appendix for those readers who are interested in rigorous derivations.

Proposition 1 says that although C is an orthogonal array of strength two, many of its four-column subarrays in fact have strength four. Though not relevant to the objective of this article, it is at least mathematically interesting to note that Proposition 1 can be generalized in a number of ways. For instance, if A is still of strength two but B is of strength three, then any six-column subarray of the resulting C obtained by taking three columns from one group and three columns from another group is an orthogonal array of strength six.

2.2. Design Construction and Orthogonality

Using Proposition 1, we now reorganize the columns of $C = (C_1, C_2, \ldots, C_{m_1})$ as in (2) into sets of four columns, each being an $OA(n, p^4, 4)$. To ensure there are no leftover columns, let both m_2 and $m_1 m_2/2$ be even, and write $m_2 = 2k$. This means that m_1 can be any integer if m_2 is a multiple of 4 and m_1 has to be even if m_2 is even but not a multiple of 4. For the $m_2 = 2k$ columns in each group C_i, we form k pairs of columns by writing C_i as

$$C_i = (P_{i1}, P_{i2}, \ldots, P_{ik}), \text{ for } i = 1, \ldots, m_1,$$

where each pair P_{ij} is composed of two columns from group C_i, and altogether $P_{i1}, P_{i2}, \ldots, P_{ik}$ exhaust all the $m_2 = 2k$ columns of C_i. Now order the $m_1 k$ pairs as

$$P_{11}, P_{21}, \ldots, P_{m_1 1}, P_{12}, P_{22}, \ldots, P_{m_1 2}, \ldots, P_{1k}, P_{2k}, \ldots, P_{m_1 k}. \quad (3)$$

Since any two successive pairs in the above list are from different groups, if we take two pairs at a time in the order given in (3), we obtain q sets of four columns, each of which is an $OA(n, p^4, 4)$, where $q = m_1 k/2 = m_1 m_2/4$. Let these sets be $C^{(1)}, C^{(2)}, \ldots, C^{(q)}$ and further let

$$C^* = (C^{(1)}, C^{(2)}, \ldots, C^{(q)}). \quad (4)$$

It is seen that C^* and C consist of the same set of $m_1 m_2$ columns; while the columns in C are in m_1 groups of size m_2 with the property as described in Proposition 1, the columns of C^* are in q sets of size 4, each being an $OA(n, p^4, 4)$, where $q = m_1 m_2/4$. Now define

$$D^* = (C^{(1)} R, C^{(2)} R, \ldots, C^{(q)} R), \quad (5)$$

where

$$R = \begin{bmatrix} p^3 & -p^2 & -p & 1 \\ p^2 & p^3 & -1 & -p \\ p & -1 & p^3 & -p^2 \\ 1 & p & p^2 & p^3 \end{bmatrix}, \quad (6)$$

which is a rotation matrix up to a constant.

Theorem 1. Design D^* constructed above and given in (5) is an $OD(n, (p^4)^m)$, an orthogonal design for $m = m_1 m_2$ factors, each with p^4 levels, and becomes an orthogonal Latin hypercube when $n = s^2$ and $s = p^2$.

Unlike the method in Steinberg and Lin (2006) and Pang, Liu, and Lin (2009), our construction method requires no use of finite fields and projective geometries, and in particular does not require s and p to be primes or prime powers. Moreover, our method can construct a richer class of orthogonal designs than orthogonal Latin hypercubes. When the starting arrays A and B both have index unity, the resulting design D^* is an orthogonal

Latin hypercube. When one or more of the starting arrays A and B do not have index unity, our method is still applicable, resulting in an orthogonal design with many levels. To illustrate these generalities, we give three applications of our method.

Application 1. Take A as an OA $(s^{k_1}, s^{(s^{k_1}-1)/(s-1)}, 2)$ and B as an OA $(s, p^{(p^{k_2}-1)/(p-1)}, 2)$ where p is a prime or prime power and $s = p^{k_2}$. Both arrays are from the Rao–Hamming construction (Hedayat, Sloane, and Stufken 1999, sec. 3.4). To apply our method, one column may need to be deleted from A or B or both to make both m_2 and $m_1m_2/2$ even. An application of our method then gives rise to an OD$(n, (p^4)^m)$, an orthogonal design of $n = s^{k_1}$ runs for $m = m_1m_2$ factors, each with p^4 levels, where $m_1 = (s^{k_1}-1)/(s-1)$ or $(s^{k_1}-1)/(s-1)-1$ and $m_2 = (p^{k_2}-1)/(p-1)$ or $(p^{k_2}-1)/(p-1)-1$. When $k_1 = k_2 = 2$, both arrays A and B have index unity, the resulting orthogonal design is an orthogonal Latin hypercube. For one example, taking $p = 3$ and $k_1 = k_2 = 2$, we obtain an orthogonal Latin hypercube of 81 runs for 40 factors. For another example, taking $p = 3$, $k_1 = 3$, and $k_2 = 2$, we obtain an OD$(729, 81^{364})$. In both examples, no deletion of a column from A or B is necessary as $B = \text{OA}(9, 3^4, 2)$ already has $m_2 = 4$, a multiple of 4.

Application 2. Take B as in Application 1, and take A as an OA$(2s^{k_1}, s^{2(s^{k_1}-1)/(s-1)-1}, 2)$, which is from the Addelman–Kempthorne construction (Hedayat, Sloane, and Stufken 1999, sec. 3.3). Then our method generates an OD$(n, (p^4)^m)$, an orthogonal design of $n = 2s^{k_1}$ runs for $m = m_1m_2$ factors, each with p^4 levels, where $m_1 = 2(s^{k_1}-1)/(s-1)-1$ or $2(s^{k_1}-1)/(s-1)-2$ and $m_2 = (p^{k_2}-1)/(p-1)$ or $(p^{k_2}-1)/(p-1)-1$. For $p = 3$ and $k_1 = k_2 = 2$, we obtain an OD$(162, 81^{76})$.

Application 3. Take A as an OA$(n, s^{m_1}, 2)$ and B as an OA$(s, 2^{m_2}, 2)$, where s is a multiple of 4, and both m_2 and $m_1m_2/2$ are even. An application of our method gives an OD$(n, 16^m)$ where $m = m_1m_2$. For one example, if we take A as an OA$(144, 12^7, 2)$ and B as an OA$(12, 2^8, 2)$, we obtain an OD$(144, 16^{56})$. For another example, let A be an OA$(144, 12^6, 2)$ and B an OA$(12, 2^{10}, 2)$, we obtain an OD$(144, 16^{60})$. If an orthogonal design of 144 runs for 56 factors is required by a computer experiment, we can use the first design directly or the second design with four columns deleted. The two choices both end up using orthogonal designs of 144 runs for 56 factors each with 16 levels, but the two designs actually have different space-filling properties, a topic to be examined in the next section.

2.3. Space-Filling Properties

The designs constructed in Section 2.2 have some attractive space-filling properties, which we will study next. For any column c of C^* in (4), by inspecting the form of matrix R in (6), we see that the column d of D^* in (5) that corresponds to c has the following form:

$$d = cp^3 \pm c'p^2 \pm c''p \pm c''', \tag{7}$$

where c and c' are in the same pair and so are c'' and c''', and up to a column permutation (c, c', c'', c''') is $C^{(j)}$ for some $j = 1, \dots, q$. Henceforth, if two columns are in the same pair, we say that one is the companion of the other. Therefore, for example, c' is the companion of c and vice versa.

Consider the mapping

$$f(x) = \left\lceil \frac{x + (p^4-1)/2}{p^3} \right\rceil - (p-1)/2 \qquad \text{for } x \in \Omega(p^4), \tag{8}$$

which collapses the p^4 levels in $\Omega(p^4)$ into the p levels in $\Omega(p)$, where $\Omega(s)$ represents the s centered equally spaced levels as given in (1). For example, with $p = 2$, collapsing the 16 levels into 2 levels by this mapping works as follows:

$$\begin{array}{ccccccccc} -7.5, & -6.5, & -5.5, & -4.5, & -3.5, & -2.5, & -1.5, & -0.5 & \longrightarrow -0.5 \\ 0.5, & 1.5, & 2.5, & 3.5, & 4.5, & 5.5, & 6.5, & 7.5 & \longrightarrow 0.5. \end{array}$$

For $p = 3$, we have

$$\begin{array}{cccccccccc} -40, & -39, & -38, & \dots, & -16, & -15, & -14 & \longrightarrow & -1 \\ -13, & \dots, & -1, & 0, & 1, & \dots, & 13 & \longrightarrow & 0 \\ 14, & 15, & 16, & \dots, & 38, & 39, & 40 & \longrightarrow & 1. \end{array}$$

Remark 1. The mapping for level collapsing in (8) is not as intuitive as one would like. This is all because of centering in our use of the levels. If the s levels were chosen as $0, 1, \dots, s-1$, then collapsing p^4 levels into p levels could be simply done using the mapping $\lceil x/p^3 \rceil$. The two extra terms $(p^4-1)/2$ and $(p-1)/2$ are needed in (8) so as to take care of the centered levels.

With the mapping in (8) and by recalling that like C, design C^* is an OA$(n, p^m, 2)$, the following result is obtained.

Proposition 2. Design D^* in (5) becomes design C^* in (4) after level collapsing as given in (8), which means that D^*, as an orthogonal design of p^4 levels, achieves a stratification on a $p \times p$ grid in any two dimension.

Proposition 2 is established if we can show that d becomes c after level collapsing by (8), that is, $f(d) = c$, where d and c are as in (7). A proof of this is given in the appendix. Steinberg and Lin (2006) presented a special case of Proposition 2. This space-filling property, though not discussed in Pang, Liu, and Lin (2009), also holds for their designs. We next establish a much stronger space-filling property for our designs.

Consider two columns d_1 and d_2 of D^*. By (7), they can be written as

$$\begin{aligned} d_1 &= c_1p^3 \pm c_1'p^2 \pm c_1''p \pm c_1''' \quad \text{and} \\ d_2 &= c_2p^3 \pm c_2'p^2 \pm c_2''p \pm c_2''', \end{aligned} \tag{9}$$

where as before c_1' is the companion of c_1 and c_2' is the companion of c_2 and so on. Now we collapse the p^4 levels in $\Omega(p^4)$ of d_1 and d_2 into the p^2 levels $\Omega(p^2)$ using the mapping

$$g(x) = \left\lceil \frac{x + (p^4-1)/2}{p^2} \right\rceil - (p^2-1)/2 \qquad \text{for } x \in \Omega(p^4). \tag{10}$$

For $p = 2$, by $g(x)$, the 16 levels are mapped into the 4 levels according to

$$\begin{array}{rrrrcr} -7.5, & -6.5, & -5.5, & -4.5 & \longrightarrow & -1.5 \\ -3.5, & -2.5, & -1.5, & -0.5 & \longrightarrow & -0.5 \\ 0.5, & 1.5, & 2.5, & 3.5 & \longrightarrow & 0.5 \\ 4.5, & 5.5, & 6.5, & 7.5 & \longrightarrow & 1.5. \end{array}$$

Then we must have

$$g(d_1) = c_1 p \pm c_1' \quad \text{and} \quad g(d_2) = c_2 p \pm c_2'. \tag{11}$$

There are three possible cases for the four columns (c_1, c_1', c_2, c_2').

(i) c_1 and c_2 are in the same pair. Then $(c_1, c_1', c_2, c_2') = (c_1, c_2, c_2, c_1)$.

(ii) c_1 and c_2 are not in the same pair but belong to the same group C_i for some $i = 1, \ldots, m_1$, where C_i as in (2) is the group of m_2 columns resulting from replacing the ith column of A by the rows of B. In this case, the four columns c_1, c_1', c_2, c_2', though distinct, are all from the same group C_i, since c_1' and c_2' are the companions of c_1 and c_2, respectively.

(iii) c_1 and c_2 are from two different groups. In this case, the two pairs (c_1, c_1') and (c_2, c_2') are also from two different groups. Then by Proposition 1, (c_1, c_1', c_2, c_2') is an $\mathrm{OA}(n, p^4, 4)$.

It is this case (iii) that gives a stronger space-filling property. After the level collapsing by (10), the two-column matrix (d_1, d_2) becomes $(g(d_1), g(d_2)) = (c_1 p \pm c_1', c_2 p \pm c_2')$, which must be an $\mathrm{OA}(n, (p^2)^2, 2)$, a p^2 level array of strength 2 because (c_1, c_1', c_2, c_2') is an $\mathrm{OA}(n, p^4, 4)$.

Let D be the design obtained by arranging the columns of D^* according to the original grouping of the columns of C. Whereas the order of the columns of D^* follows that of C^*, the order of the columns of D follows that of C. This way, the columns of D are in m_1 groups of size m_2 just like C. Corresponding to (2), we write

$$D = (D_1, D_2, \ldots, D_{m_1}), \tag{12}$$

where D_i corresponds to C_i. We are ready to present the next theorem.

Theorem 2. Design D as (12) achieves a stratification on a $p^2 \times p^2$ grid in any two dimension provided that the two columns are from different groups D_{i_1} and D_{i_2} with $i_1 \neq i_2$.

By Proposition 2 and Theorem 2, we see that design D achieves a stratification on a $p \times p$ grid in all two dimensions and it achieves a stratification on a finer $p^2 \times p^2$ grid in those two dimensions given by two columns from different groups. The proportion of the two dimensions with this stronger space-filling property is given by

$$\pi = (m_1 - 1)m_2/(m_1 m_2 - 1), \tag{13}$$

which is very high and in fact close to 1 so long as m_1 is not too small. For example, for the $\mathrm{OD}(81, 81^{40})$ and the $\mathrm{OD}(729, 81^{364})$ obtained in Application 1, we have that $\pi = 36/39 = 12/13$ and $\pi = 360/363 = 120/121$, respectively.

The properties of design D described in Proposition 2 and Theorem 2 are reminiscent of the notion of mappable nearly orthogonal arrays recently introduced and studied by Mukerjee, Sun, and Tang (2014). A mappable nearly orthogonal array $\mathrm{MNOA}(n; (s^{m_2})^{m_1}, (p^{m_2})^{m_1})$ is an array of n runs for $m_1 m_2$ factors each with s levels that has m_1 groups of m_2 factors such that any two columns form an $\mathrm{OA}(n, s^2, 2)$ if they are from different groups, and can be collapsed into an $\mathrm{OA}(n, p^2, 2)$ if they are from the same group. Using this definition, we see that design D becomes an $\mathrm{MNOA}(n; (s^{m_2})^{m_1}, (p^{m_2})^{m_1})$ where $s = p^2$ if the p^4 levels are collapsed into p^2 levels. In other words, D, an orthogonal design of p^4 levels, has an underlying structure of an $\mathrm{MNOA}(n; (s^{m_2})^{m_1}, (p^{m_2})^{m_1})$ where $s = p^2$. Note that our D and an $\mathrm{MNOA}(n; (s^{m_2})^{m_1}, (p^{m_2})^{m_1})$ with $s = p^2$ are two different designs notwithstanding their similar space-filling properties in two dimensions. The former has p^4 levels whereas the latter has p^2 levels; the former is an orthogonal design whereas the latter is not.

In Table 1, we provide some new orthogonal designs that can be constructed using our method. The space-filling properties of these designs are characterized using their underlying mappable nearly orthogonal arrays in the table.

Of special interest are orthogonal Latin hypercubes constructible by our method, some of which are listed in Table 2, where again their space-filling properties are described by their underlying mappable nearly orthogonal arrays. Here familiar notation $\mathrm{OLH}(n, m)$ is used to represent an orthogonal Latin hypercube of n runs for m factors. The orthogonal Latin hypercubes in Table 2 are new because of their space-filling properties. The previous methods (Steinberg and Lin 2006; Pang, Liu, and Lin 2009) allow construction of an $\mathrm{OLH}(16, 12)$, an $\mathrm{OLH}(81, 40)$, an $\mathrm{OLH}(625, 156)$, and an $\mathrm{OLH}(2401, 400)$ but these designs only guarantee stratifications on $p \times p$ grids in

Table 1. Some orthogonal designs and their space-filling properties.

p	Array A	Array B	Orthogonal design D	Space-filling properties
2	$\mathrm{OA}(32, 4^8, 2)$	$\mathrm{OA}(4, 2^2, 2)$	$\mathrm{OD}(32, 16^{16})$	$\mathrm{MNOA}(32; (4^2)^8, (2^2)^8)$
2	$\mathrm{OA}(64, 4^{20}, 2)$	$\mathrm{OA}(4, 2^2, 2)$	$\mathrm{OD}(64, 16^{40})$	$\mathrm{MNOA}(64; (4^2)^{20}, (2^2)^{20})$
2	$\mathrm{OA}(64, 8^8, 2)$	$\mathrm{OA}(8, 2^6, 2)$	$\mathrm{OD}(64, 16^{48})$	$\mathrm{MNOA}(64; (4^6)^8, (2^6)^8)$
2	$\mathrm{OA}(128, 8^{16}, 2)$	$\mathrm{OA}(8, 2^6, 2)$	$\mathrm{OD}(128, 16^{96})$	$\mathrm{MNOA}(128; (4^6)^{16}, (2^6)^{16})$
2	$\mathrm{OA}(144, 12^6, 2)$	$\mathrm{OA}(12, 2^{10}, 2)$	$\mathrm{OD}(144, 16^{60})$	$\mathrm{MNOA}(144; (4^{10})^6, (2^{10})^6)$
2	$\mathrm{OA}(144, 12^7, 2)$	$\mathrm{OA}(12, 2^8, 2)$	$\mathrm{OD}(144, 16^{56})$	$\mathrm{MNOA}(144; (4^8)^7, (2^8)^7)$
3	$\mathrm{OA}(162, 9^{19}, 2)$	$\mathrm{OA}(9, 3^4, 2)$	$\mathrm{OD}(162, 81^{76})$	$\mathrm{MNOA}(162; (9^4)^{19}, (3^4)^{19})$
3	$\mathrm{OA}(729, 9^{91}, 2)$	$\mathrm{OA}(9, 3^4, 2)$	$\mathrm{OD}(729, 81^{364})$	$\mathrm{MNOA}(729; (9^4)^{91}, (3^4)^{91})$
3	$\mathrm{OA}(648, 18^{18}, 2)$	$\mathrm{OA}(18, 3^6, 2)$	$\mathrm{OD}(648, 81^{108})$	$\mathrm{MNOA}(648; (9^6)^{18}, (3^6)^{18})$
4	$\mathrm{OA}(512, 16^{33}, 2)$	$\mathrm{OA}(16, 4^4, 2)$	$\mathrm{OD}(512, 256^{132})$	$\mathrm{MNOA}(512; (16^4)^{33}, (4^4)^{33})$
5	$\mathrm{OA}(1250, 25^{50}, 2)$	$\mathrm{OA}(25, 5^6, 2)$	$\mathrm{OD}(1250, 625^{300})$	$\mathrm{MNOA}(1250; (25^6)^{50}, (5^6)^{50})$

Table 2. Some orthogonal Latin hypercubes and their space-filling properties.

p	Array A	Array B	OLH(n, m)	Space-filling properties	π
2	OA$(16, 4^4, 2)$	OA$(4, 2^2, 2)$	OLH$(16, 8)$	MNOA$(16;\ (4^2)^4, (2^2)^4)$	0.857
3	OA$(81, 9^{10}, 2)$	OA$(9, 3^4, 2)$	OLH$(81, 40)$	MNOA$(81;\ (9^4)^{10}, (3^4)^{10})$	0.923
4	OA$(256, 16^{17}, 2)$	OA$(16, 4^4, 2)$	OLH$(256, 68)$	MNOA$(256;\ (16^4)^{17}, (4^4)^{17})$	0.955
5	OA$(625, 25^{26}, 2)$	OA$(25, 5^6, 2)$	OLH$(625, 156)$	MNOA$(625;\ (25^6)^{26}, (5^6)^{26})$	0.968
7	OA$(2401, 49^{50}, 2)$	OA$(49, 7^8, 2)$	OLH$(2401, 400)$	MNOA$(2401;\ (49^8)^{50}, (7^8)^{50})$	0.982

two dimensions with $p = 2, 3, 5, 7$, respectively. The orthogonal Latin hypercubes OLH$(16, 8)$, OLH$(81, 40)$, OLH$(625, 156)$, and OLH$(2401, 400)$ in Table 2 from our method achieve stratifications on $p^2 \times p^2$ grids in most of two dimensions in addition to being space-filling on $p \times p$ grids in all two dimensions, where $p = 2, 3, 5, 7$, respectively. Table 2 provides this information through π, defined in (13) to be the proportion of the two dimensions that are space-filled on $p^2 \times p^2$ grids. For $n = 256$, the method of Steinberg and Lin (2006) can construct an OLH$(256, 248)$, which has a very high factor-to-run ratio. On the other hand, their design only promises stratifications on 2×2 grids in two dimensions. Our design OLH$(256, 68)$ in Table 2 has a smaller factor-to-run ratio but enjoys much better space-filling properties—it achieves stratifications on 16×16 grids in 2176 out of 2278 two dimensions and on 4×4 grids in the remaining 102 two dimensions.

3. Further Results

This section revisits Lin, Mukerjee, and Tang (2009). Our method in Section 2 is partially inspired by the method of Lin, Mukerjee, and Tang (2009). As a payback, we now use the ideas of the former to extend the application scope of the latter.

In a nutshell, the method of Lin, Mukerjee, and Tang (2009) constructs a large orthogonal Latin hypercube from a small orthogonal Latin hypercube using an orthogonal array with an even number of factors. With some adjustments, we present a version of the method that will allow the construction of a large orthogonal design from a small orthogonal design using an orthogonal array with its number of factors not necessarily even.

Let A be an OA$(n, s^{m_1}, 2)$ as in Section 2, but let B be an OD(s, p^{m_2}). Again we replace the uth level in each column of A by the uth row of B and let $C = (C_1, C_2, \ldots, C_{m_1})$ denote the resulting array as before, where C_i is the ith group of m_2 factors from replacing the levels in the ith column of A by the rows of B. Though not an OA$(n, p^{m_1 m_2}, 2)$, the resulting array C is still an OD$(n, p^{m_1 m_2})$. Analogous to Proposition 1, we have the following simple result.

Lemma 1. Any two columns from different groups C_{i_1} and C_{i_2} where $i_1 \neq i_2$ must form an OA$(n, p^2, 2)$, a strength two array.

Now suppose that $m_1 m_2$ is even and let $m_1 m_2/2 = q$. Then Lemma 1 will allow us to reorganize the $m_1 m_2$ columns of C into q sets of two columns such that each set of two columns gives an OA$(n, p^2, 2)$. This is done as follows. Let $c_{i1}, \ldots, c_{im_2}$ be the columns of C_i. Thus,

$$C = (c_{11}, \ldots, c_{1m_2}; c_{21}, \ldots, c_{2m_2}; \ldots; c_{m_1 1}, \ldots, c_{m_1 m_2}).$$

Note that any two consecutive columns in the following ordered list:

$$c_{11}, c_{21}, \ldots, c_{m_1 1}; c_{12}, c_{22}, \ldots, c_{m_1 2}; \ldots; c_{1m_2}, c_{2m_2}, \ldots, c_{m_1 m_2} \quad (14)$$

are from different groups. Thus, if we take two columns at a time in the order given by (14), we obtain $q = m_1 m_2/2$ sets of two columns, each being an OA$(n, p^2, 2)$. Let these sets be $C^{(1)}, \ldots, C^{(q)}$ and $C^* = (C^{(1)}, \ldots, C^{(q)})$. Then we see that

$$D^* = (C^{(1)}R, \ldots, C^{(q)}R), \quad \text{where } R = \begin{pmatrix} p & -1 \\ 1 & p \end{pmatrix}$$

is an OD$(n, (p^2)^m)$ where $m = m_1 m_2$. Like before, we rearrange the columns of D^* according to the order of columns in C, and let

$$D = (D_1, \ldots, D_{m_1}), \quad (15)$$

where the columns of D_i can be regarded as the rotated columns of C_i. Note that D becomes C if its p^2 levels are collapsed into p levels according to

$$h(x) = \left\lceil \frac{x + (p^2 - 1)/2}{p} \right\rceil - (p - 1)/2 \qquad \text{for } x \in \Omega(p^2).$$

We summarize the above results in a proposition.

Proposition 3. Design D constructed above and given in (15) is an OD$(n, (p^2)^{m_1 m_2})$ and achieves a stratification on a $p \times p$ grid in any two dimension provided that the two columns are from different groups D_{i_1} and D_{i_2} with $i_1 \neq i_2$.

Compared with the original version in Lin, Mukerjee, and Tang (2009), the above version has two new aspects. One is that B can be any orthogonal design, which is not necessarily an orthogonal Latin hypercube. This may be trivial mathematically but recognizing the fact and making it explicit allow a richer class of orthogonal designs to be constructed. The other is that we only need to assume $m_1 m_2$ is even whereas Lin, Mukerjee, and Tang (2009) assumed an even m_1. Obviously, the new case of odd m_1 and even m_2 is now covered. Table 3 presents what we can accomplish with our improved method by constructing some orthogonal Latin hypercubes that are not previously available. For a comparison, the corresponding orthogonal Latin hypercubes that can be constructed from the original method of

Table 3. Some orthogonal Latin hypercubes from our improved method.

Array A	Array B	Improved LMT	Original LMT
OA$(64, 8^9)$	OLH$(8, 4)$	OLH$(64, 36)$	OLH$(64, 32)$
OA$(144, 12^7)$	OLH$(12, 8)$	OLH$(144, 56)$	OLH$(144, 48)$
OA$(256, 16^{17})$	OLH$(16, 12)$	OLH$(256, 204)$	OLH$(256, 192)$
OA$(1024, 32^{33})$	OLH$(32, 16)$	OLH$(1024, 528)$	OLH$(1024, 512)$

Lin, Mukerjee, and Tang (2009) are given in the last column of the table. We see that the orthogonal Latin hypercubes from our method all have more columns than those given by the original method. It is noteworthy that the OLH(256, 204) in Table 3 offers an appealing compromise between the OLH(256, 68) in Table 2 and the OLH(256, 248) of Steinberg and Lin (2006) if both the factor-to-run ratio and space-filling properties are important to an experimenter. Finally, we note that in Table 3 the OLH(8, 4) is from Ye (1998), the OLH(12, 8) from Georgiou (2009), the OLH(16, 12) from Steinberg and Lin (2006), and the OLH(32, 16) is from Sun, Liu, and Lin (2009).

4. Summary and Discussion

A general method is presented in Section 2 that allows the construction of a rich class of space-filling orthogonal designs. The method can construct orthogonal Latin hypercubes as well as other orthogonal designs. Compared to Steinberg and Lin (2006) and Pang, Liu, and Lin (2009), our method is simple as it does not require the use of finite fields and projective geometries. The most salient feature of our method is its space-filling properties, producing orthogonal designs that achieve much better stratifications in low-dimensional projections. The ideas of our construction in Section 2 are then used in Section 3 to obtain an improved version of the method of Lin, Mukerjee, and Tang (2009), making it more flexible in the choices of base arrays.

Table 1 in Section 2 provides some orthogonal designs constructible using our method. These designs are all new as there has not been a previous method available that allows the construction of orthogonal designs with space-filling properties. In Table 2 of Section 2, we list some orthogonal Latin hypercubes obtained by our method. Orthogonal Latin hypercubes with similar parameters can also be constructed using the previous methods (Steinberg and Lin 2006; Pang, Liu, and Lin 2009) but they only promise a weak space-filling property. In contrast, the orthogonal Latin hypercubes in Table 2 from our method guarantee a much stronger space-filling property. Compared to the original method of Lin, Mukerjee, and Tang (2009), our improved version in Section 3 can construct orthogonal Latin hypercubes with more columns, some of which are tabulated in Table 3.

For a given set of parameters n, s, m_1, p, m_2, our method in Sections 2 can be used to generate a family of space-filling orthogonal designs. Nonisomorphic choices of A and B lead to different versions of the final design D. Even for given A and B, one can permute the levels in each column of array C before the action of rotating-in-groups to obtain different final designs D. All these final designs have the same orthogonality property as stated in Theorem 1 and the same space-filling properties as guaranteed by Proposition 2 and Theorem 2. The availability of these different versions of design D provides us with an opportunity of finding better ones using some secondary design criteria. With respect to orthogonality, one can further evaluate these designs using three-orthogonality (Bingham, Sitter, and Tang 2009), which provides a measure for the robustness of linear effect estimates to second-order effects. As for the space-filling property, distance or discrepancy criteria may be used for design selection. Compared to the minimax distance criterion, the maximin distance criterion is more convenient to use as its evaluation depends only on the design points but not on other points in the design region (Johnson, Moore, and Ylvisaker 1990). Among the many existing discrepancy criteria, the centered L_2 discrepancy is very attractive (Hickernell 1998). A full investigation of further evaluating our space-filling orthogonal designs based on some secondary criteria described above is out of scope for this article. Nonetheless, this represents an important direction we will look at in the future. Finally, we note that similar studies for Latin hypercubes and OA-based Latin hypercubes were previously carried out by Morris and Mitchell (1995) and Leary, Bhaskar and Keane (2003), respectively.

Appendix: Proofs

Proof of Proposition 1. Without loss of generality, we only need to consider C_1 and C_2. Let a_1, a_2 be the first two columns of A. Thus, C_i where $i = 1, 2$ is obtained by replacing the uth level of a_i by the uth row of B for every $u = 1, \dots, s$. Let c_i, d_i be any two columns of C_i for $i = 1, 2$. As A is an $\mathrm{OA}(n, s^{m_1}, 2)$, each pair (u_1, u_2) where $u_1, u_2 \in \Omega(s)$ occurs λ_1 times as a row in matrix (a_1, a_2), where $n = \lambda_1 s^2$. Since B is an $\mathrm{OA}(s, p^{m_2}, 2)$, each pair (v_1, v_2) where $v_1, v_2 \in \Omega(p)$ occurs λ_2 times as a row in any submatrix of two columns of B, where $s = \lambda_2 p^2$. Thus, each pair (v_1, v_2), as a row of matrix (c_1, d_1), must meet each pair (v_1', v_2'), as a row of matrix (c_2, d_2), $\lambda_1\lambda_2^2$ times in the rows of (c_1, d_1, c_2, d_2), where $v_1, v_2, v_1', v_2' \in \Omega(p)$. In other words, each four-tuple (v_1, v_2, v_1', v_2') where $v_1, v_2, v_1', v_2' \in \Omega(p)$ must occur $\lambda_1\lambda_2^2$ times in the rows of (c_1, d_1, c_2, d_2). This establishes that (c_1, d_1, c_2, d_2) is an $\mathrm{OA}(n, p^4, 4)$. □

Proof of Theorem 1. The orthogonality of design D^* follows from the facts that R is an orthogonal matrix and that C^*, as an OA of strength 2, is an orthogonal design. From Pang, Liu, and Lin (2009), it is known that if $C^{(j)}$ is a full p^4 factorial of single replicate, then $C^{(j)}R$ is a design with each of the four factors having equally spaced p^4 levels in $\Omega(p^4)$. In our case, each $C^{(j)}$ is an $\mathrm{OA}(n, p^4, 4)$, which is a full p^4 factorial of $n/(p^4)$ replicates. Therefore, each of the four factors in $C^{(j)}R$ must also have equally spaced p^4 levels in $\Omega(p^4)$, all repeated $n/(p^4)$ times. This completes the proof. □

Proof of Proposition 2. We only need to show that $f(d) = c$, the meaning of which is that d becomes c after f is applied to every component of d. In the following derivations, $f(d)$ is to be interpreted as we are working with any given component of d. We now have

$$f(d) = \left[\frac{cp^3 \pm c'p^2 \pm c''p \pm c''' + (p^4-1)/2}{p^3}\right] - (p-1)/2$$
$$= \left[\frac{b_1p^3 + b_2p^2 + b_3p + b_4}{p^3}\right] - (p-1)/2,$$

where $b_1 = c + (p-1)/2$, $b_2 = \pm c' + (p-1)/2$, $b_3 = \pm c'' + (p-1)/2$, and $b_4 = \pm c''' + (p-1)/2$. As the entries of $(c, \pm c', \pm c'', \pm c''')$ are all in $\Omega(p)$, the entries of (b_1, b_2, b_3, b_4) must all take values in $\{0, 1, \dots, p-1\}$. This means that $b_2p^2 + b_3p + b_4$ must have values less than p^3. We therefore have $f(d) = b_1 - (p-1)/2 = c$, as desired. □

Proof of Theorem 2. That $g(d_1) = c_1p \pm c_1'$ and $g(d_2) = c_2p \pm c_2'$ as in (11) can be proved in the same way as we prove $f(d) = c$ for Proposition 2. What remains to be shown is that $(g(d_1), g(d_2))$ is an $\mathrm{OA}(n, (p^2)^2, 2)$. This can be seen to be true from the following:

(a) since (c_1, c_1', c_2, c_2') is an $\mathrm{OA}(n, p^4, 4)$ taking levels from $\Omega(p)$, $(c_1, \pm c_1', c_2, \pm c_2')$ is also an $\mathrm{OA}(n, p^4, 4)$ taking levels from $\Omega(p)$;

(b) because of (a), each pair (v_1, v_1'), as a row of $(c_1, \pm c_1')$, must meet each pair (v_2, v_2'), as a row of $(c_2, \pm c_2')$, $\lambda = n/(p^4)$ times in the rows of $(c_1, \pm c_1', c_2, \pm c_2')$, where $v_1, v_1', v_2, v_2' \in \Omega(p)$;

(c) $x_1p + x_2$ establishes a one-to-one correspondence between the p^2 pairs (x_1, x_2) where $x_1, x_2 \in \Omega(p)$ and the p^2 levels in $\Omega(p^2)$. □

Funding

The research of Fasheng Sun is supported by the National Natural Science Foundation of China. The research of Boxin Tang is supported by the Natural Sciences and Engineering Research Council of Canada.

References

Bingham, D., Sitter, R. R., and Tang, B. (2009), "Orthogonal and Nearly Orthogonal Designs for Computer Experiments," *Biometrika*, 96, 51–65. [683,688]

Box, G. E., and Draper, N. R. (1959), "A Basis for the Selection of a Response Surface Design," *Journal of the American Statistical Association*, 54, 622–654. [683]

Cheng, C. S., Steinberg, D. M., and Sun, D. X. (1999), "Minimum Aberration and Model Robustness for Two-Level Fractional Factorial Designs," *Journal of the Royal Statistical Society*, Series B, 61, 85–93. [684]

Fang, K. T., Li, R. Z., and Sudjianto, A. (2006), *Design and Modeling for Computer Experiments*, New York: Chapman & Hall. [683]

Georgiou, S. D. (2009), "Orthogonal Latin Hypercube Designs From Generalized Orthogonal Designs," *Journal of Statistical Planning and Inference*, 139, 1530–1540. [688]

——— (2011), "Orthogonal Designs for Computer Experiments," *Journal of Statistical Planning and Inference*, 141, 1519–1525. [683]

He, Y., and Tang, B. (2013), "Strong Orthogonal Arrays and Associated Latin Hypercubes for Computer Experiments," *Biometrika*, 100, 254–260. [683]

Hedayat, A. S., Sloane, N. J. A., and Stufken, J. (1999), *Orthogonal Arrays: Theory and Applications*, New York: Springer. [684,685]

Hickernell, F. (1998), "A Generalized Discrepancy and Quadrature Error Bound," *Mathematics of Computation of the American Mathematical Society*, 67, 299–322. [688]

Johnson, M., Moore, L., and Ylvisaker, D. (1990), "Minimax and Maximin Distance Designs," *Journal of Statistical Planning and Inference*, 26, 131–148. [683,688]

Joseph, V. R., and Hung, Y. (2008), "Orthogonal-Maximin Latin Hypercube Designs," *Statistica Sinica*, 18, 171–186. [683]

Leary, S., Bhaskar, A., and Keane, A. (2003), "Optimal Orthogonal-Array-Based Latin Hypercubes," *Journal of Applied Statistics*, 30, 585–598. [688]

Lin, C. D., Bingham, D., Sitter, R. R., and Tang, B. (2010), "A New and Flexible Method for Constructing Designs for Computer Experiments," *Annals of Statistics*, 38, 1460–1477. [683]

Lin, C. D., Mukerjee, R., and Tang, B. (2009), "Construction of Orthogonal and Nearly Orthogonal Latin Hypercubes," *Biometrika*, 96, 243–247. [683,687,688]

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. [683]

Morris, M. D., and Mitchell, T. J. (1995), "Exploratory Designs for Computational Experiments," *Journal of Statistical Planning and Inference*, 43, 381–402. [688]

Mukerjee, R., Sun, F., and Tang, B. (2014), "Nearly Orthogonal Arrays Mappable Into Fully Orthogonal Arrays," *Biometrika*, 101, 957–963. [683,686]

Owen, A. B. (1992), "Orthogonal Arrays for Computer Experiments, Integration, and Visualization," *Statistica Sinica*, 2, 439–452. [683]

Pang, F., Liu, M. Q., and Lin, D. K. (2009), "A Construction Method for Orthogonal Latin Hypercube Designs With Prime Power Levels," *Statistica Sinica*, 19, 1721–1728. [683,684,685,686,688]

Sacks, J., and Ylvisaker, D. (1984), "Some Model Robust Designs in Regression," *Annals of Statistics*, 12, 1324–1348. [683]

Santner, T. J., Williams, B. J., and Notz, W. I. (2003), *The Design and Analysis of Computer Experiments*, New York: Springer. [683]

Steinberg, D. M., and Lin, D. K. J. (2006), "A Construction Method for orthogonal Latin Hypercube Designs," *Biometrika*, 93, 279–288. [683,684,685,686,688]

Sun, F., Liu, M. Q., and Lin, D. K. (2009), "Construction of Orthogonal Latin Hypercube Designs," *Biometrika*, 96, 971–974. [683,688]

Tang, B. (1993), "Orthogonal Array-Based Latin Hypercubes," *Journal of American Statistical Association*, 88, 1392–1397. [683]

Ye, K. Q. (1998), "Orthogonal Column Latin Hypercubes and Their Application in Computer Experiments," *Journal of American Statistical Association*, 93, 1430–1439. [683,688]