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A note on orthogonal Latin hypercubes

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Abstract

Latin hypercube designs have been found very useful for designing computer experiments. In recent years, several methods of constructing orthogonal Latin hypercube designs have been proposed in the literature. In this article, we report some more results on Latin hypercube designs, including several new designs.

Keywords: Latin hypercube designs; orthogonal arrays.

1. Introduction

Latin hypercube designs introduced by McKay *et al.* (1979) have proved to be a popular choice of experimental design when computer simulation is used for studying a physical process as the design points of a Latin hypercube are equally spaced in the design region when projected onto univariate margins. A Latin hypercube design, LH(n, m), is an $n \times m$ matrix whose columns are permutations of the column vector $(1, 2, ..., n)'$. Some times, it is convenient to visualize a Latin hypercube design in its centered form. For a positive integer n, let $\boldsymbol{g}_n$ be an $n \times 1$ vector with its ith element equal to $(i - (n+1)/2)$, $1 \leq i \leq n$, and G_n be the set of all permutations of $\boldsymbol{g}_n$. A centered Latin hypercube design is an $n \times m$ matrix with columns from G_n. The columns of a Latin hypercube design represent the input factors and, the rows, the experimental runs. Different approaches have been suggested in the literature for constructing Latin hypercubes with desirable properties. One such approach consists of finding Latin hypercubes with zero correlations between pairs of input factors (or, columns). In terms of centered Latin hypercube designs, this requirement is equivalent to the condition that

(a) the columns of the design are mutually orthogonal.

Designs satisfying condition (a) are called orthogonal Latin hypercubes (OLH) and will henceforth be denoted by $\text{OLH}_1(n, m)$. An $\text{OLH}_1(n, m)$ design ensures independence of estimates of linear effects when a first order

model is fitted. However, if a second-order model is needed, then it is desirable that the Latin hypercube design satisfies condition (a) and additionally, the following condition:
(b) the element-wise square of each column and the element-wise product of every two columns are orthogonal to all columns in the design.

A Latin hypercube design with n rows and m columns satisfying both (a) and (b) will be denoted by $\mathrm{OLH}_2(n, m)$. An $\mathrm{OLH}_2(n, m)$ design ensures that not only the estimates of linear effects are mutually uncorrelated but they are also are uncorrelated with the estimates of quadratic and interaction effects in a second order model. In recent years, construction of Latin hypercube designs satisfying either (a) or both (a) and (b) has received considerable attention. Several families of $\mathrm{OLH}_1(n, m)$ designs were reported by Steinberg and Lin (2006), Lin *et al.* (2009) and Pang *et al.* (2009). In particular, Lin *et al.* (2009) gave a method of construction of a large $\mathrm{OLH}_1(n, m)$ design by combining a smaller $\mathrm{OLH}_1(n, m)$ design with a suitable orthogonal array of strength two.

Quite a few families of $\mathrm{OLH}_2(n, m)$ designs are available in the literature. The values of n and m for these $\mathrm{OLH}_2(n, m)$ designs are given below, where $u \geq 1$ is an integer:

(i) $n = 2^{u+1},\ m = 2u$ and $n = 2^{u+1} + 1,\ m = 2u$; Ye (1998).
(ii) $n = 2^{u+1},\ m = u + 1 + \binom{u}{2}$ and $n = 2^{u+1} + 1,\ m = u + 1 + \binom{u}{2}$, $u \leq 11$; Cioppa and Lucas (2007).
(iii) $n = 2^{u+1},\ m = 2^u$ and $n = 2^{u+1} + 1,\ m = 2^u$; Sun *et al.* (2009).
(iv) $n = r2^{u+1},\ m = 2^u$ and $n = r2^{u+1} + 1,\ m = 2^u$, $r \geq 1$ being an integer; Sun *et al.* (2010).

Georgiou (2009) obtained some $\mathrm{OLH}_1(n, m)$ and $\mathrm{OLH}_2(n, m)$ designs, using orthogonal and generalized orthogonal designs. Sun *et al.* (2009) observed that in a (centered) Latin hypercube design $\mathrm{OLH}_2(n, m)$, $m \leq [n/2]$, where $[x]$ is the integer part of x. Clearly, the designs of Sun *et al.* (2009) with parameters as in (iii) above attain this upper bound.

In this note, we present some more results on orthogonal Latin hypercubes. All the available $\mathrm{OLH}_1(n, m)$ and $\mathrm{OLH}_2(n, m)$ designs with *even* n are such that $n \equiv 0 \pmod 4$. We show that if $n \equiv 2 \pmod 4$, then there does not exist an $\mathrm{OLH}_1(n, m)$ design (and, consequently, an $\mathrm{OLH}_2(n, m)$ design). We also extend a result of Lin *et al.* (2009) on the construction of a large $\mathrm{OLH}_1(n, m)$ design by combining a smaller $\mathrm{OLH}_1(n, m)$ design with an orthogonal array of strength two. Using this extended version, several new

$\mathrm{OLH}_1(n,m)$ designs are obtained.

For n *odd*, apart from the families with parameters (i)–(iv) above, Lin *et al.* (2009) using a computer search reported two OLHs, viz., an $\mathrm{OLH}_1(7,3)$ and an $\mathrm{OLH}_1(11,7)$. Pang *et al.* (2009) also presented several $\mathrm{OLH}_1(n,m)$ designs, where $n = p^d$ and $m = (p^d-1)/(p-1)$, $p \geq 3$ is a prime and d is a power of 2. We report two $\mathrm{OLH}_1(n,m)$ designs with n odd, viz., an $\mathrm{OLH}_1(13,7)$ and an $\mathrm{OLH}_1(15,6)$, neither of which can be constructed by the existing methods. We also report three new $\mathrm{OLH}_2(n,m)$ designs, viz., an $\mathrm{OLH}_2(11,3)$, an $\mathrm{OLH}_2(13,3)$ and an $\mathrm{OLH}_2(15,4)$. The first and third designs with $n=11$ and $n=15$ rows cannot be constructed by the existing methods and the second design is an improvement over an existing design.

2. Existence and construction of $\mathrm{OLH}_1(n,m)$ designs

We first prove the following result.

Lemma. *If* $n \equiv 2 \pmod 4$ *then there does not exist an* $\mathrm{OLH}_1(n,m)$.

Proof. If possible, let there exist an $\mathrm{OLH}_1(n,m)$ where $n \equiv 2 \pmod 4$. Consider an arbitrary pair of columns, $\boldsymbol{x} = (x_1,\ldots,x_n)'$ and $\boldsymbol{y} = (y_1,\ldots,y_n)'$ of this $\mathrm{OLH}_1(n,m)$, each of which is a permutation of $(1,2,\ldots,n)'$. By the hypothesis, $\boldsymbol{x}$ and $\boldsymbol{y}$ are uncorrelated and thus we must have

$$\sum_{i=1}^{n} x_i y_i = n^{-1}\left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right). \tag{1}$$

Since $\sum_{i=1}^{n} x_i = n(n+1)/2 = \sum_{i=1}^{n} y_i$, the right side of (1) equals $n(n+1)^2/4$, which is not an integer if $n \equiv 2 \pmod 4$. But the left side of (1) is necessarily an integer. Thus (1) cannot hold. $\square$

It follows then that a necessary condition for the existence of an $\mathrm{OLH}_1(n,m)$ design with even n is that $n \equiv 0 \pmod 4$.

We next present an extension of a result of Lin *et al.* (2009). Let A be an orthogonal array $OA(n^2,p,n,2)$ with n^2 rows, p columns, n symbols, strength 2 and index unity and B be an orthogonal Latin hypercube design, $\mathrm{OLH}_1(n,q)$ with n rows and q columns, such that $pq(=2u)$ is an even integer. Without loss of generality, let the symbols of A be $1,2,\ldots,n$. For $1 \leq j \leq q$, let A_j be a $n^2 \times p$ matrix obtained by replacing in A, the symbols $1,2,\ldots,n$ by the 1st, 2nd, $\ldots$,nth entry in the jth column of B. Partition $[A_1\ A_2\ \cdots A_q]$ as $[A_1^*\ A_2^* \cdots A_u^*]$, where for $1 \leq j \leq u$, A_j^* has two columns.

Define $V = \begin{bmatrix} 1 & -n \\ n & 1 \end{bmatrix}$ and let $M_j = A_j^* V$. Consider the $n^2 \times 2u$ matrix $M = [M_1\ M_2 \cdots M_u]$. We then have the following result.

Theorem. *The existence of an orthogonal array $OA(n^2, p, n, 2)$ and an* $\mathrm{OLH}_1(n, q)$ *design such that pq is an even integer implies the existence of an* $\mathrm{OLH}_1(n^2, pq)$ *design.*

Proof. It is not hard to see that M is a Latin hypercube design in the sense that each of it columns is a member of G_n, where G_n is as in Section 1. Now, observe that $M = [A_1^*V\ A_2^*V \cdots A_u^*V] = [A_1^*\ A_2^* \cdots A_u^*](I_u \otimes V)$, where $\otimes$ denotes the tensor product. Therefore, $M'M = (I_u \otimes V')(C'C)(I_u \otimes V)$, where $C = [A_1^*\ A_2^* \cdots A_u^*]$. Now, the two columns in any A_j^* arise either from (i) the same column of B or, (ii) from two distinct columns of B. If p is even, case (ii) does not arise and the pairwise orthogonality of the columns of C and hence that of M follows from the fact that A is an orthogonal array of strength two. Suppose p is odd (and, hence q is necessarily even). In such a case, if the two columns in A_j^* arise from the same column of B, the pairwise orthogonality of the columns of M again follows as above. If the two columns of A_j^* arise from two distinct columns of B, the same orthogonality holds, because the columns of B are mutually orthogonal. This completes the proof. □

Note that Lin *et al.* (2009) start with an orthogonal array of strength two with *even* number of columns and thus, the requirement in the theorem that pq be even is automatically satisfied. As we shall see in the next section, the extended result as given above, allows us to construct several new $\mathrm{OLH}_1(n, m)$ designs, not covered by the construction of Lin *et al.* (2009).

3. Some new orthogonal Latin hypercube designs

We first make an application of the theorem in obtaining some new $\mathrm{OLH}_1(n, m)$ designs. Combining an $\mathrm{OLH}_1(8, 4)$ of Ye (1998), an $\mathrm{OLH}_1(12, 8)$ of Georgiou (2009) and an $\mathrm{OLH}_1(16, 12)$ of Steinberg and Lin (2006) respectively, with an $OA(64, 9, 8, 2)$, an $OA(144, 7, 12, 2)$ and an $OA(256, 17, 16, 2)$ and invoking the theorem, one obtains an $\mathrm{OLH}_1(64, 36)$, an $\mathrm{OLH}_1(144, 56)$ and an $\mathrm{OLH}_1(256, 204)$, all of which appear to be new. Each of these designs has a better column-to-row ratio than the ones given by the construction of Lin *et al.* (2009), namely, an $\mathrm{OLH}_1(64, 32)$, an $\mathrm{OLH}_1(144, 48)$ and an $\mathrm{OLH}_1(256, 192)$.

We now consider orthogonal Latin hypercube designs with n odd. Georgiou (2009) claimed that one can construct an $\mathrm{OLH}_1(13,8)$ using Corollary 2 of his paper. This claim does not appear to be correct as Corollary 2 in Georgiou (2009) cannot lead to an $\mathrm{OLH}_1(13,8)$. However, through a computer search, it has been possible to obtain an $\mathrm{OLH}_1(13,7)$, which is shown in Table 1 in centered form. In Table 1, we also show an $\mathrm{OLH}_1(15,6)$. Combining the $\mathrm{OLH}_1(13,7)$ design in Table 1 with an orthogonal array OA(169,14,13,2), we obtain a new $\mathrm{OLH}_1(169,98)$, which has many more columns than that in the $\mathrm{OLH}_1(169,14)$, reported by Pang *et al.* (2009). Similarly, combining the $\mathrm{OLH}_1(15,6)$ with an orthogonal array $OA(225,6,15,2)$ leads to an $\mathrm{OLH}_1(225,36)$.

Table 1. *Orthogonal Latin hypercubes* $\mathrm{OLH}_1(13,7)$ and $\mathrm{OLH}_1(15,6)$

$\mathrm{OLH}_1(13,7)$

−6	−1	−6	−2	−5	−1	−5
−5	6	0	1	1	−3	4
−4	2	4	−3	6	0	−4
−3	−3	−2	−5	−2	6	5
−2	−2	6	2	−4	2	3
−1	−6	3	5	5	4	−2
0	0	−4	3	4	−4	6
1	1	1	−1	2	−5	−3
2	−4	2	4	−6	−6	−1
3	3	−1	0	−1	3	−6
4	4	−5	6	0	5	0
5	5	5	−4	−3	1	2
6	−5	−3	−6	3	−2	1

$\mathrm{OLH}_1(15,6)$

−7	−1	−2	−5	−5	−1
−6	6	−1	7	6	−5
−5	5	2	1	−4	−6
−4	−4	5	−3	1	4
−3	−3	7	−4	3	1
−2	−2	−7	5	−7	6
−1	−7	−6	2	4	−2
0	0	0	0	7	2
1	1	1	−7	−3	0
2	2	−5	−1	−2	3
3	3	3	3	2	7
4	4	4	4	−1	5
5	−5	−4	−2	5	−3
6	−6	6	6	−6	−7
7	7	−3	−6	0	−4

In Table 2, we show three Latin hypercube designs, an $\mathrm{OLH}_2(11,3)$, an $\mathrm{OLH}_2(13,3)$ and an $\mathrm{OLH}_2(15,4)$. The first and third Latin hypercube designs in Table 2 cannot be constructed by the existing methods, while the second one has one more column than in an $\mathrm{OLH}_2(13,2)$, obtained by following the method of Sun *et al.* (2010). Furthermore, a computer search shows that a Latin hypercube design with 11 or 13 rows and satisfying (a) and (b) can have no more than 3 columns.

Table 2. *Orthogonal Latin hypercubes* $\mathrm{OLH}_2(11,3)$, $\mathrm{OLH}_2(13,3)$ *and* $\mathrm{OLH}_2(15,4)$

$\mathrm{OLH}_2(11,3)$			$\mathrm{OLH}_2(13,3)$			$\mathrm{OLH}_2(15,4)$			
						−7	−7	−1	−3
			−6	3	−4	−6	6	−4	−4
−5	−5	−1	−5	−5	−3	−5	5	6	6
−4	3	−2	−4	−4	6	−4	−4	5	1
−3	1	5	−3	6	2	−3	3	−2	−2
−2	4	−3	−2	2	5	−2	−2	−3	5
−1	2	4	−1	1	−1	−1	−1	−7	7
0	0	0	0	0	0	0	0	0	0
5	5	1	6	−3	4	1	1	7	−7
4	−3	2	5	5	3	2	2	3	−5
3	−1	−5	4	4	−6	3	−3	2	2
2	−4	3	3	−6	−2	4	4	−5	−1
1	−2	−4	2	−2	−5	5	−5	−6	−6
			1	−1	1	6	−6	4	4
						7	7	1	3

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