Orthogonal Latin Hypercube Designs for Two and Three Factors

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Abstract

In this article, we give a complete solution to the construction problem of second order orthogonal Latin hypercube designs for any number of runs for two and three factors by combining smaller orthogonal Latin hypercube designs.

Keywords: Latin hypercube designs, orthogonal, computer experiments

1 Introduction

In many scientific and engineering research investigations, physical experimentation is often very expensive and quite time consuming. In such situations, a practical approach is to describe the physical systems by mathematical equations. One can simulate the system by finding numerical solutions to these equations. Such type of experiments are called computer experiments. Latin hypercube designs introduced by McKay et al. (1979) have become most popular in computer experiments. A Latin hypercube design with n runs and m factors is represented by an $n \times m$ matrix, where each column is a uniform permutation of n equally spaced levels $1, 2, 3, ..., n$. The levels of each factor may be represented in its centered form. In other words, for odd n, the levels $1, 2, ..., i, ..., n$ are represented as $-(n-1)/2, -(n-1)/2+1, ..., -(n-1)/2+(i-1), ..., (n-1)/2-1, (n-1)/2$. For even n, the levels $1, 2, ..., n$ are represented as $-(n-1), -(n-3), ..., -(n-1)+2(i-1), ..., (n-3), (n-1)$. Clearly, in the centered form, when n is even, half of the levels are positive and half of the levels are negative and for odd n, half of the levels are positive, half are negative and one level is at 0.

A Latin hypercube design is said to be an orthogonal Latin hypercube design if correlation between any two columns is zero. When the levels are represented in its centered form, an orthogonal Latin hypercube design has the property that the inner product of any two columns is zero. When a first-order model is fitted, an orthogonal Latin hypercube design ensures the independence of estimates of linear effects. Hence, such designs are also called

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first order orthogonal Latin hypercube designs, which we denote as OLH_1 designs. However, sometimes second order models may be fitted. In such situations, second order orthogonal Lain hypercube designs are desirable. A Latin hypercube design is said to be second order orthogonal if it satisfies the conditions of an OLH_1 design and the condition that the element-wise square of each column and the element-wise product of every two columns are orthogonal to all columns in the design. We shall denote a second order Latin hypercube designs as OLH_2 design. Clearly, for existence of an OLH_2 design, it is necessary that an OLH_1 design exists. However, vice versa is not true.

A lot of work has been done to construct orthogonal Latin hypercube designs. Ye (1998) proposed a method to construct OLH_2 designs with (a) $n = 2^{r+1} + 1$ and $m = 2r$ (b) $n = 2^{r+1}$ and $m = 2r$ for any integer $r \geq 1$. Steinberg and Lin (2006) provided a method of construction of OLH_1 designs for 2^{2^r} run sizes for any integer r. Cioppa and Lucas (2007) extended Ye's construction to obtain more columns for (a) $n = 2^{r+1} + 1$ and $m = \binom{r}{2} + r + 1$ (b) $n = 2^{r+1}$ and $m = \binom{r}{2} + r + 1$. Pang et al. (2009) developed a method of construction of OLH_1 designs for p^{2^r} runs and up to $(p^{2^r} - 1)/(p - 1)$ factors by rotating groups of factors in a p-level p^{2^r}-run regular fractional factorial designs, where p is a prime. Nguyen (2008) and Sun et al. (2009) independently introduced OLH_2 designs for (a) $2^{r+1} + 1$ runs in 2^r factors and (b) 2^{r+1} runs in 2^r factors for any integer $r \geq 1$. Sun et al. (2010) obtained a method of construction of OLH_2 designs for $s2^{r+1} + 1, s2^{r+1}$ runs and 2^r factors for all integer $s \geq 1$. Lin et al. (2009) proposed a method for construction of OLH_2 designs using orthogonal designs. Lin et al. (2010) developed a method for construction of OLH_1 designs and nearly orthogonal designs which are more flexible as compared to existing methods with respect to factor-run combinations. They also proved that no OLH_1 design exists when $n = 4r + 2$ with r being a positive integer. Dey and Sarkar (2014) gave a new result on construction of OLH_1 designs using orthogonal arrays and provided some new OLH_2 designs, for example, 11 runs with 3 factors, 13 runs with 3 factors through computer aided search.

Although, the literature is enriched with a number of construction methods for orthogonal Latin hypercube designs but most of them are for some specific runs and specific factors and hence, there are gaps in the parameters for construction of orthogonal Latin hypercubes. For example, method of Ye (1998); Cioppa and Lucas (2007); Sun et al. (2009) and Sun et al. (2010) fail to construct orthogonal Latin hypercube designs of $6, 7, 11, 12, 13, 15, 19, 20, 21$ runs. In this paper, we address the construction problem of OLH_2 designs for two and three factors for any number of runs.

2 Methods of Construction

First we state the following existing result due to Lin et al. (2010).

Lemma 1. There exists no OLH_1 designs with n runs and m factors when $n = 4r + 2$ for any positive integer r.

An elegant proof of Lemma 1 is given by Dey and Sarkar (2014). Lemma 1 implies that an OLH_2 design also does not exist for $n = 4r + 2$ runs. Next, we note the following trivial result.

Table 1: An OLH_1 design for $n = 7, m = 3$

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

Lemma 2. There exists no OLH_1 and OLH_2 designs with $m = 3$ factors for $n = 3, 4$ and 5 runs.

Lemma 2 can be easily verified by an exhaustive search in computer. Thus, to have an OLH_1 and OLH_2 design for $m = 3$ factors, we need $n \geq 7$ runs, since $n = 6$ is covered by Lemma 1. We prove here that there exists no OLH_2 design for $n = 7$ and $m = 3$. To see this, without loss of generality, assume that the first column is given by $\mathbf{c}_1 = (-3, -2, -1, 0, 1, 2, 3)'$. It can be found by exhaustive computer search that there are four possible columns $\mathbf{c}_2$ which satisfy the conditions $\mathbf{c}_1'\mathbf{c}_2 = 0$ and $(\mathbf{c}_1^2)'\mathbf{c}_2 = 0$ where $\mathbf{c}_1^2$ denotes the column obtained by squaring each of the elements of $\mathbf{c}_1$. These four columns are $(0, 2, -3, -1, 1, 3, -2)'$, $(2, -3, -1, 1, 3, -2, 0)'$, $(0, -2, 3, 1, -1, -3, 2)'$ and $(-2, 3, 1, -1, -3, 2, 0)'$. However, none of the four columns satisfy $(\mathbf{c}_2^2)'\mathbf{c}_1 = 0$. Therefore, an OLH_2 design does not exist for $n = 7, m = 3$. However, an OLH_1 design for $n = 7, m = 3$ exists and one such design is given in Table 1.

We shall call a matrix $\mathbf{A} = (\mathbf{a}_1, ..., \mathbf{a}_m)$ as second order orthogonal if (a) $\mathbf{a}_i'\mathbf{a}_j = 0$ for any $i \neq j = 1, 2, ..., m$, (b) $\mathbf{a}_i'(\mathbf{a}_j \circ \mathbf{a}_k) = 0$ for any $i \neq j \neq k = 1, 2, ..., m$ and (c) $(\mathbf{a}_i^2)'\mathbf{a}_j = 0$ and $(\mathbf{a}_j^2)'\mathbf{a}_i = 0$ for any $i \neq j = 1, 2, ..., m$. Here, $\circ$ denote the Hadamard product. Clearly, a second order orthogonal matrix $\mathbf{A}$ is an OLH_2 design if each of the columns $\mathbf{a}_i, i = 1, 2, ...m$ contains each of the levels of the factors exactly once. Now, we present a result for constructing a second order orthogonal matrix for $m = 3$ with $n = 8r$ runs.

Theorem 1. Let $\pm a_i, \pm b_i, \pm c_i, \pm d_i, i = 1, 2, ..., r$ be any $8r$ real numbers such that none of them is 0. Consider the matrix $\mathbf{D} = (\mathbf{D}_1', \mathbf{D}_2', ..., \mathbf{D}_r')'$ with

$$\mathbf{D}_i = \begin{pmatrix} \mathbf{B}_i \\ -\mathbf{B}_i \end{pmatrix} \text{ with } \mathbf{B}_i = \begin{pmatrix} a_i & c_i & d_i \\ b_i & d_i & -c_i \\ c_i & -a_i & b_i \\ d_i & -b_i & -a_i \end{pmatrix}. \tag{2.1}$$

Then, the $\mathbf{D}$ is a second order orthogonal matrix and each column of the matrix $\mathbf{D}$ contains each of the numbers $\pm a_i, \pm b_i, \pm c_i, \pm d_i, i = 1, 2, ..., r$ exactly once.

Now, we present methods for constructing OLH_2 designs for $m = 3$ for all n for which an OLH_2 design exists. Any run size n can fall into one of these six cases for which an OLH_2 design with $m = 3$ can exist:

I) $n = 8r$,

II) $n = 8r + 1$,

III) $n = 8r + 3$,

IV) $n = 8r + 4$,

V) $n = 8r + 5$ and

VI) $n = 8r + 7$

where r is a positive integer. For $n = 8r + 2 = 4r^* + 2$ with $r^* = 2r$ and hence, an OLH_2 design does not exist for any m by Lemma 1. Similarly, for $n = 8r + 6 = 4r^* + 2$ with $r^* = 2r + 1$, an OLH_2 design does not exist for any m.

Case I: In Theorem 1, let $a_i, b_i, c_i, d_i, i = 1, 2, ..., r$, represent the $4r$ positive (or negative) levels of the factors. Then, the matrix $\mathbf{D}$ is an OLH_2 design with $8r$ runs and 3 factors.

Example 1. Let $r = 1$. Then, $n = 8$ and the levels of the factors may be represented as $-7, -5, -3, -1, 1, 3, 5, 7$. Let $a_1 = -7, b_1 = -5, c_1 = -3, d_1 = -1$. Then, the matrix

$$\mathbf{D} = \begin{pmatrix} -7 & -3 & -1 \\ -5 & -1 & 3 \\ -3 & 7 & -5 \\ -1 & 5 & 7 \\ 7 & 3 & 1 \\ 5 & 1 & -3 \\ 3 & -7 & 5 \\ 1 & -5 & -7 \end{pmatrix}$$

is an OLH_2 design.

Case II: For $n = 8r+1$, let the $8r+1$ levels of the factors be $-4r, -4r+1, ..., -1, 0, 1, ..., 4r-1, 4r$. Using Theorem 1, we can construct a second order orthogonal matrix $\mathbf{D}$ from the $8r$ non-zero levels. Adding a row of zeros, we get an OLH_2 design with $n = 8r + 1$ runs and $m = 3$ factors.

Case III: For $n = 8r+3$, with $r = 1$, an OLH_2 design for 11 runs is given by Dey and Sarkar (2014) and is given in Table 2(a). For $r > 1$, the levels of each factor can be partitioned into two sets $S_1 = \{-5, -4, ..., -1, 0, 1, ..., 4, 5\}$ and $S_2 = \{-4r-1, -4r, ..., -7, -6, 6, 7, ..., 4r, 4r+1\}$ of sizes 11 and $8(r-1)$, respectively. From 11 levels in set S_1, we can get a second order orthogonal matrix (say $\mathbf{D}_1$) as in Table 2(a). Using Theorem 1, we can construct a second order orthogonal matrix $\mathbf{D}_2$ with $8(r-1)$ rows and 3 columns from the levels in set S_2. Juxtaposing the matrices $\mathbf{D}_1$ and $\mathbf{D}_2$ gives an OLH_2 design with $n = 8r + 3$ runs for $r > 1$.

Case IV: When $n = 8r + 4$, for $r = 1$, an OLH_2 design for 12 runs is obtained by deleting the center point from an OLH_2 design with 13 runs given in Table 2(c) and then centering the levels for even n. The resulting OLH_2 design for 12 runs is displayed in Table 2(b). For $r > 1$, Theorem 1 gives a second order orthogonal matrix $\mathbf{D}_2$ with $8(r-1)$ runs from $8(r-1)$ levels $\{-8r-3, -8r-1, ..., -13, 13, ..., 8r+1, 8r+3\}$. Combining the design in Table 2(b) with $\mathbf{D}_2$, we get an OLH_2 design with $n = 8r + 4$ runs for $r > 1$.

Table 2: Smaller Second Order Orthogonal Latin Hypercube Designs with Three Factors

(a) $n = 11$

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

(b) $n = 12$

−11	5	−7
−9	−9	−5
−7	−7	11
−5	11	3
−3	3	9
−1	1	−1
11	−5	7
9	9	5
7	7	−11
5	−11	−3
3	−3	−9
1	−1	1

(c) $n = 13$

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

(d) $n = 15$

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

Case V: For $n = 8r + 5$, with $r = 1$, an OLH_2 design for 13 runs due to Dey and Sarkar (2014) is given in Table 2(c). For $r > 1$, Theorem 1 gives a second order orthogonal matrix $\mathbf{D}_2$ with $8(r-1)$ runs from $8(r-1)$ levels $\{-4r-2, -4r-1, ..., -7, 7, ..., 4r+1, 4r+2\}$. Combining the design in Table 2(c) with $\mathbf{D}_2$, we get an OLH_2 design with $n = 8r + 5$ runs.

Case VI: For $n = 8r + 7$, when $r = 0$, we have already presented an OLH_1 design for 7 runs in Table 1 and proved that no OLH_2 design exists for 7 runs with $m = 3$. For $r = 1$, an OLH_2 design for 15 runs is given in Table 2(d) and is due to Dey and Sarkar (2014). For $r > 1$, Theorem 1 can be utilized to construct an orthogonal matrix $\mathbf{D}_2$ with $8r - 1$ runs from $8(r-1)$ levels $\{-4r-3, -4r-2, ..., -8, 8, ..., 4r+2, 4r+3\}$. Combining the design in Table 2(d) with $\mathbf{D}_2$, an OLH_2 design with $n = 8r + 7$ runs can be obtained for $r > 1$.

2.1 Orthogonal Latin Hypercube Designs for Two Factors

Two OLH_2 designs for $n = 4$ and 5 for $m = 2$ factors given by Ye (1998) are given in Table 3. For constructing an OLH_2 design with $n > 6$ runs and $m = 2$ factors, one can delete any one column from an OLH_2 design with n runs and $m = 3$ factors. Thus, the construction problem for OLH_2 designs for any runs for $m = 2$ is also solved.

3 Concluding Remarks

A number of methods are available in literature for construction of orthogonal Latin hypercube designs. Most of the methods are for some specific runs and for specific factors. Methods of Ye (1998); Cioppa and Lucas (2007); Sun et al. (2009, 2010) fail to construct orthogonal Latin hypercube designs for runs 7,11, 12,13,15,19,20,21,23,24,..., with three factors. In this article, the construction problem of second order orthogonal Latin hypercube

Table 3: Smaller Orthogonal Latin Hypercube Designs for Two Fators

(a) $n = 4$

−3	−1
−1	3
1	−3
3	1

(b) $n = 5$

−2	−1
−1	2
0	0
1	−2
2	1

designs in terms of runs sizes has been completely solved for three and two factors. Further research efforts are being made to obtain orthogonal Latin hypercube designs for higher number of columns for any run size. The work will be communicated in a separate article.

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