



## A Note on Second Order Orthogonal Latin Hypercube Designs

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### SUMMARY

Latin hypercube designs (LHDs) are commonly used in designing computer experiments. In recent years, several methods of constructing orthogonal Latin hypercube designs have been proposed in the literature. In this article, two new series of second order orthogonal Latin hypercube designs for six factors have been given.

*Keywords:* Latin hypercube designs, Orthogonal, Second order, Computer experiments.

### 1. INTRODUCTION

Latin hypercube designs (LHDs), proposed by McKay *et al.*, 1979, are widely adopted in the designing of computer experiments with quantitative factors because they spread the design points uniformly in any one-dimensional projection. An LHD with  $n$  runs and  $m$  factors is denoted by a matrix, where  $L(n, m) = (l_1, \dots, l_m)$  is  $l_j, j = 1, 2, \dots, m$  the  $j^{\text{th}}$  factor, and each factor includes  $n$  uniformly spaced levels  $\{1, 2, \dots, n\}$ . Often it is convenient to present the levels of the factors in an LHD in its centered form. To be specific, the levels belong to the set  $\{-(n-1)/2, -(n-3)/2, \dots, -(n-2i+1)/2, \dots, (n-3)/2, (n-1)/2\}$ . We denote the set as  $\mathcal{L}$ .

An LHD when represented in its centered form is called an orthogonal LHD if the inner product of any two distinct columns is zero. Henceforth, we denote an orthogonal Latin hypercube design with  $n$  runs and  $m$  factors as an OLH  $(n, m)$ . As discussed in Sun *et al.*, 2009, an OLH ensures that the parameter estimates of the first order polynomial model

$$y = \beta_0 + \sum_{j=1}^m \beta_j x_j + \varepsilon \quad (1)$$

are uncorrelated. Recently, considerable attention is being given to the parameter estimation of second

order polynomial model

$$y = \beta_0 + \sum_{j=1}^m \beta_j x_j + \sum_{j=1}^m \beta_{jj} x_j^2 + \sum_{j=1}^{m-1} \sum_{j_1=j+1}^m \beta_{jj_1} x_j x_{j_1} + \varepsilon. \quad (2)$$

When model (2) is used along with an OLH, it is desirable that the OLH should ensure that there is no correlation between parameter estimates of first and second order effects. This requires that the OLH should have the additional properties that (a) the entry-wise square of each column is orthogonal to all columns in the design and (b) the entry-wise product of any two distinct columns is orthogonal to all columns in the design. Such an OLH is called as second order OLH. Clearly, a second order OLH is always an OLH but an OLH may not be a second order OLH. Henceforth, unless we mention the words “second order”, an OLH will simply refer to first order OLH. Several workers have given a number of methods of construction of OLHs for different  $n$  and  $m$ . The values of  $n$  and  $m$  for which second order OLHs are available in literature are given in the following list.

1.  $n = 2^{k+1}, m = 2k$  and  $n = 2^{k+1} + 1, m = 2k$  and [Ye, 1998]

2.  $n = 2^{k+1}, m = k + 1 + \binom{k}{2}$  and  $n = 2^{k+1} + 1, m = k + 1 + \binom{k}{2}, k \leq 11$  (Cioppa & Lucas, 2007)
3.  $n = 2^{k+1}, m = 2^k$  and  $n = 2^{k+1} + 1, m = 2^k$  [Sun *et al.*, 2009]
4.  $n = r2^{k+1}, m = 2^k$  and  $n = r2^{k+1} + 1, m = 2^k$  [Sun *et al.*, 2010]
5.  $n = 11, 13, m = 3$  and  $n = 15, m = 4$  [Dey and Sarkar, 2014]
6.  $n = s \text{ mod } 8, s = 0, 1, 3, 5, 7, m = 3$  [Parui *et al.*, 2016]
7.  $n = 0, 1 \text{ mod } 8, m \leq 4$  and  $n = 0, 1 \text{ mod } 16, m \leq 8$  [Evangelaras and Koutras, 2017] where  $k \geq 1$  is an integer.

Lin *et al.* (2010), Georgiou and Efthimiou (2014), Mandal *et al.* (2016), Dey and Sarkar (2017) and Sun and Tang (2017) provided several interesting construction methods for OLHs.

In spite of the above works for constructing OLH designs, there are many run sizes for which a construction method of OLH, particularly for second order OLHs, does not exist. For example, the above methods do not allow construction of second order OLHs for  $n = 56, 57$  runs for any  $m$ . In this article, we give two new series of second order OLHs up to six factors with  $n = 16r + q$  with  $r$  being a positive integer and  $q = 8$  or  $9$ .

## 2. METHODS OF CONSTRUCTION

To construct new second order OLH designs for six factors, we make use of second order orthogonal matrices. We shall call an  $n \times m$  matrix  $A = (a_1', \dots, a_m')$  as second order orthogonal if

1.  $a_i' a_j = 0$  for all  $i \neq j = 1, 2, \dots, m$ ,
2.  $(a_i^2)' a_j = 0$  and  $(a_j^2)' a_i = 0$  for all  $i \neq j = 1, 2, \dots, m$  and
3.  $(a_i \circ a_j)' a_k = 0$  for all  $i \neq j \neq k = 1, 2, \dots, m$  where  $\circ$  denote the Hadamard product.

We denote a second order orthogonal matrix with  $n$  rows and  $m$  columns as  $OM_2(n, m)$ . Now, we present a result for constructing an  $OM_2(n, 6)$  with  $n \equiv 0 \text{ mod } 16$ .

Let  $\pm a_i, \pm b_i, \pm c_i, \pm d_i, \pm e_i, \pm f_i, \pm g_i, \pm h_i, i = 1, 2, \dots, t$  be any  $16t$  real numbers such that none of them is 0 where  $t$  is a positive integer. Consider the matrix with

$$D = (D_1', D_2', \dots, D_t')'$$

$$D_i = \begin{pmatrix} H_i \\ -H_i \end{pmatrix}$$

$$H_i = \begin{bmatrix} a_i & -b_i & -d_i & -c & -h_i & e_i \\ b_i & a_i & -c_i & d_i & -g_i & -f_i \\ c_i & -d_i & b_i & a_i & -f_i & g_i \\ d_i & c_i & a_i & -b_i & -e_i & -h_i \\ e_i & -f_i & -h & g_i & d_i & -a_i \\ f_i & e_i & -g_i & -h_i & c_i & b_i \\ g_i & -h_i & f_i & -e_i & b_i & -c_i \\ h_i & g_i & e_i & f_i & a_i & d_i \end{bmatrix} \quad (3)$$

Then, the  $D$  is a  $OM_2(16t, 6)$  and each column of the matrix  $D$  contains each of the numbers  $\pm a_i, \pm b_i, \pm c_i, \pm d_i, \pm e_i, \pm f_i, \pm g_i, \pm h_i, i = 1, 2, \dots, t$  exactly once.

Lemma 1 is very useful to construct  $OM_2(16t, 6)$ . We give an example of constructing an  $OM_2(16, 6)$ .

**Example 1:** Let  $t = 1$  in Lemma 1 and set  $a_1 = 25/2, b_1 = 27/2, c_1 = 29/2, d_1 = 31/2, e_1 = 33/2, f_1 = 35/2, g_1 = 37/2, h_1 = 39/2$ . Then the matrix

$$D = \frac{1}{2} \begin{bmatrix} 25 & -27 & -31 & -29 & -39 & 33 \\ 27 & 25 & -29 & 31 & -37 & -35 \\ 29 & -31 & 27 & 25 & -35 & 37 \\ 31 & 29 & 25 & -27 & -33 & -39 \\ 33 & -35 & -39 & 37 & 31 & -25 \\ 35 & 33 & -37 & -39 & 29 & 27 \\ 37 & -39 & 35 & -33 & 27 & -29 \\ 39 & 37 & 33 & 35 & 25 & 31 \\ -25 & 27 & 31 & 29 & 39 & -33 \\ -27 & -25 & 29 & -31 & 37 & 35 \\ -29 & 31 & -27 & -25 & 35 & -37 \\ -31 & -29 & -25 & 27 & 33 & 39 \\ -33 & 35 & 39 & -37 & -31 & 25 \\ -35 & -33 & 37 & 39 & -29 & -27 \\ -37 & 39 & -35 & 33 & -27 & 29 \\ -39 & -37 & -33 & -35 & -25 & -31 \end{bmatrix} \quad (4)$$

is an  $OM_2(16, 6)$ .

Note that an  $OM_2$  constructed by Lemma 1 may or may not be a second order OLH. With the proper choice of the elements  $a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, i = 1, 2, \dots, t$  in Lemma 1, a second order OLH  $(16t, 6)$  can be constructed.

**Corollary 1:** Let  $\mathbf{D}$  be a  $OM_2(16t, 6)$  as in Lemma 1. If each of the columns of the matrix  $\mathbf{D}$  contains each of the elements of  $\mathcal{L}$  exactly once, then  $\mathbf{D}$  is a second order OLH  $(16t, 6)$ .

Now, we have the following main result.

**Theorem 1:** A second order OLH  $(n, 6)$  can always be constructed for  $n \equiv 8 \pmod{16}$  with  $n \geq 24$ .

*Proof.* Let  $n = 16r + 8, r = 1, 2, \dots$ . Denote the  $n$  levels as in  $\mathcal{L}$  and arrange them in ascending order. Partition the levels into two disjoint sets  $S_1$  and  $S_2$  such that  $S_1$  contains 24 levels from the center of the arrangement and  $S_2$  contains rest of the  $16(r-1)$  levels. For the 24 levels in  $S_1$  a second order OLH  $(24, 6)$  is given Table 1. Denote this second order OLH  $(24, 6)$  as  $D_1$ . From the  $16(r-1)$  levels in  $S_2$ , construct an  $OM_2(16t, 6)$  with  $t = r - 1$  following Lemma 1 and denote it as  $D_2$ . Then, it is easy to see

that  $D = \begin{pmatrix} D_1 \\ D_2 \end{pmatrix}$  is a second order OLH  $(16r + 8, 6)$ .

We illustrate the method using an example.

**Example 2:** Consider construction of second order OLH  $(56, 6)$ . Here  $r = 3$  and  $s = 8$ . Then set  $\mathcal{L} = S_1 + S_2$  where  $S_1 = \{-23, -21, \dots, -3, -1, 1, 3, \dots, 21, 23\}$  and  $S_2 = \{-55, -53, \dots, -27, -25, 25, 27, \dots, 53, 55\}$ . An  $OM_2(32, 6)$  with elements of  $S_2$  can be easily constructed following Lemma 1 by taking  $a_1 = -55, b_1 = -53, c_1 = -51, d_1 = -49, e_1 = -47, f_1 = -45, g_1 = -43, h_1 = -41, a_2 = -39, b_2 = -37, c_2 = -35, d_2 = -33, e_2 = -31, f_2 = -29, g_2 = -27, h_2 = -25$ .

Juxtaposing  $OM_2(32, 6)$  with the second order OLH  $(24, 6)$ , we get a second order OLH  $(56, 6)$ .

**Theorem 2:** A second order OLH  $(n, 6)$  can always be constructed for  $n \equiv 9 \pmod{16}$  with  $n \geq 24$ .

*Proof.* Let  $n = 16r + 9, r = 1, 2, \dots$ . Denote the  $n$  levels as in  $\mathcal{L}$  and arrange them in ascending order. Partition the levels into two disjoint sets  $S_1$  and  $S_2$  such that  $S_1$  contains 25 levels from the center of the

arrangement and  $S_2$  contains rest of the  $16(r-1)$  levels. To obtain a second order OLH  $(25, 6)$ , multiply each element of the second order OLH  $(24, 6)$  given in Table 1 by 2 and juxtapose an additional row of zeros to the resulting matrix. Denote this second order OLH as  $D_1$ . As earlier, construct an  $OM_2(16t, 6)$  with  $t = r - 1$  following Lemma 1 from the  $16r$  levels in  $S_2$  and denote it as  $D_2$ . Then,  $D = \begin{pmatrix} D_1 \\ D_2 \end{pmatrix}$  is a second order OLH  $(16r + 9, 6)$ .

Theorem 1 and 2 give two new series of second order OLH designs for six factors and none of the existing methods can construct these second order OLHs.

**Lemma 2:** There exists no second order OLH  $(n, m)$  if  $n = 4 \pmod{8}$  for  $m \geq 3$ . Lemma 1 is due to Evangelaras and Koutras, 2017. They also showed that no second order OLH exists for  $(n, m) = \{11, 4\}, \{13, 4\}, \{15, 5\}$ . This leads immediately to the following result.

There exists no second order OLH  $(n, 6)$  for  $n = 11, 13, 15$ .

### 3. CONCLUDING REMARKS

In this article, we have presented two new series of second order OLH for  $n = s \pmod{16}, s = 8, 9$  with  $n \geq 24$ . for six factors. Further efforts are required to

**Table 1.** A second order OLH  $(24, 6)$

-23	19	-5	-17	15	21	
-21	5	-15	23	-19	17	
-19	-23	-17	5	21	-15	
-17	15	19	21	-5	-23	
-15	-17	21	-19	-23	5	
-13	-3	-1	-9	7	-11	
-11	7	-3	-13	-1	-9	
-9	-1	-7	-11	-3	-13	
-7	-11	-9	1	-13	3	
-5	-21	23	15	17	19	
-3	-13	11	7	9	-1	
$\frac{1}{2}$	-1	9	13	-3	11	7
1	-9	-13	3	-11	-7	
3	-13	-11	-7	-9	1	
5	21	-23	-15	-17	-19	
7	11	9	-1	13	-3	
9	1	-7	11	3	13	
11	-7	3	13	1	9	
13	3	1	9	-7	11	
15	17	-21	19	23	-5	
17	-15	-19	-21	5	23	
19	23	17	-5	-21	15	
21	-5	15	-23	19	-17	
23	-19	5	17	-15	-21	

obtain second order OLH designs for other values of  $n$ . The problem of construction of second order OLH  $(n,6)$  for  $n = 19,21,23,27,29$  and 31 requires attention of researchers. This will lead to complete solution of the construction problem of second order OLHs upto six factors.

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