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A new family of orthogonal Latin hypercube designs

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Summary

We present a method of construction of orthogonal Latin hypercube designs with $n = 4s + 3$ rows where s is a positive integer. All the designs constructed in this paper are believed to be new.

Some key words: Latin hypercube; Orthogonal designs; Computer experiments.

1. Introduction

Latin hypercube designs are widely used for computer experiments. A Latin hypercube design, LH(n, m), is an $n \times m$ matrix whose columns are permutations of the column vector $(1, 2, ..., n)'$. In the context of computer experiments, the columns of a Latin hypercube design represent the input factors and the rows, the experimental runs. It is some times convenient to visualize a Latin hypercube design in its centred form. For a positive integer n, let 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 g_n. A centred Latin hypercube design is an $n \times m$ matrix with columns from G_n. Henceforth, we consider Latin hypercube designs in the centred form only. A (centred) Latin hypercube design L is called orthogonal if the columns of L are mutually orthogonal.

We shall denote an orthogonal Latin hypercube design with n rows and m columns as OLH$_1(n, m)$. A subclass of OLH$_1(n, m)$ designs consists of those that satisfy the following two conditions:
(a) the entry-wise square of each column is orthogonal to all columns in the design;

(b) the entry-wise product of any two distinct columns is orthogonal to all columns in the design.

An orthogonal Latin hypercube design with n rows and m columns satisfying the conditions (a) and (b) will be denoted by $\mathrm{OLH}_2(n, m)$. Whereas an $\mathrm{OLH}_1(n, m)$ design ensures that the estimates of linear effects are mutually uncorrelated, 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.

A variety of methods of construction of $\mathrm{OLH}_1(n, m)$ and $\mathrm{OLH}_2(n, m)$ designs have been proposed in the literature. Methods of construction of $\mathrm{OLH}_1(n, m)$ designs were reported for example, by Steinberg & Lin (2006), Lin *et al.* (2009) and Lin *et al.* (2010), Georgiou (2009) and Dey & Sarkar (2016). The following families of $\mathrm{OLH}_2(n, m)$ designs are also known; in the following, $u \geq 1$ 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 & 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), Yang & Liu (2012).

Georgiou (2009) also constructed some $\mathrm{OLH}_2(n, m)$ designs using generalized orthogonal designs. Dey & Sarkar (2016) reported three new $\mathrm{OLH}_2(n, m)$ designs, obtained via computer search. Recently, Parui *et al.* (2016) produced some $\mathrm{OLH}_2(n, m)$ designs with only $m = 3$ columns, following a method similar to that of Yang & Liu (2012).

Despite the availability of several families of $\mathrm{OLH}_2(n, m)$ designs, there exist values of n for which such designs are not known, especially with more than three columns. The families of $\mathrm{OLH}_2(n, m)$ designs given in (i)–(iv) above cover the cases $n \equiv 0, 1 \pmod 4$. Also, as shown by Lin *et al.* (2010), no $\mathrm{OLH}_1(n, m)$ (and hence, $\mathrm{OLH}_2(n, m)$) design can exist if $n \equiv 2 \pmod 4$. When $n \equiv 3 \pmod 4$. Parui *et al.* (2016) constructed $\mathrm{OLH}_2(n, m)$ designs with $m = 3$. In this paper, we give a method of construction of $\mathrm{OLH}_2(n, m)$ designs with $n \equiv 3 \pmod 4$ rows and $m = 4$ or 5 columns. The method uses an orthogonal design in conjunction with an existing $\mathrm{OLH}_2(n, m)$ design.

2. The method of construction

For an integer s, let $a_s = (-x_s, -x_{s-1}, \ldots, -x_2, -x_1, x_1, x_2, \ldots, x_{s-1}, x_s)'$ be a $2s \times 1$ vector, where the x_i's are real numbers. For our purpose, we assume that no x_i equals zero. Let A be a $2s \times m$ matrix whose columns are permutations of a_s. The matrix A is called an orthogonal design if the columns of A are mutually orthogonal. Such orthogonal designs are useful in constructing orthogonal Latin hypercube designs. Four orthogonal designs with $s = 1, 2, 4, 8$ are displayed in Lin *et al.* (2010). Since we shall be using orthogonal designs with $s = 4, 8$ in our construction, we display these in Table 1.

An $\mathrm{OLH}_2(15, 4)$ design was reported by Dey & Sarkar (2016). We have now found an $\mathrm{OLH}_2(19, 5)$ design via a computer search. Both these designs are new and cannot be constructed using the existing methods. As we shall use these two designs in our construction, these are displayed in Table 2.

Remark. Note that in both the designs in Table 1, the last s rows are negatives of the first s rows. Similarly, for both the designs in Table 2, if we exclude the row of all zeros, then the last $(n-1)/2$ rows are negatives of the first $(n-1)/2$ rows. These facts are useful in the construction described below.

We first have the following result.

Lemma. *Let A_1 be an $a \times b$ matrix and $A = [A_1', \ -A_1']'$. Then, (i) the entry-wise square of each column of A is orthogonal to all columns of A and (ii) the entry-wise product of any two distinct columns of A is orthogonal to all columns of A.*

Proof. We provide a proof of (i), the proof of (ii) is similar. Let the columns of A_1 be $u_1, \ldots u_b$. Define $v_i = u_i * u_i$, $1 \leq i \leq b$, where * denotes the entry-wise (or, Hadamard) product and let $B = [v_1 v_2, \ldots, v_b]$. Then, the Hadamard product of the columns of A can be written as $[B', \ B']'$. The assertion (i) is now immediate.

We now give a method of construction of $\mathrm{OLH}_2(n, m)$ designs where $n \equiv 3 \pmod 4$.

Theorem 1. *Let $n = 4s + 3$. Then there exists an* $\mathrm{OLH}_2(4s + 3, 4)$ *design.*

Proof. We distinguish two cases according as s is odd or even.

Case 1: s odd, $s \geq 3$: When $s = 3$, we have an $\mathrm{OLH}_2(15, 4)$ shown in Table

2. Now, let $s \geq 5$. For $j = 1, 2, \ldots, (s-3)/2$, let D_j be an 8×4 matrix obtained by replacing the elements x_1, x_2, x_3 and x_4 by $8+4(j-1), 9+4(j-1), 10+4(j-1)$ and $11+4(j-1)$, respectively, in the first orthogonal design of Table 1. Also, let d_{15} be the $\mathrm{OLH}_2(15,4)$ design displayed in Table 2. Let

$$d^{(1)} = \begin{bmatrix} d_{15} \\ D_1 \\ D_2 \\ \vdots \\ D_{\frac{s-3}{2}} \end{bmatrix}.$$

Then, using the Lemma and the facts in the Remark, it is easily seen that $d^{(1)}$ is an $\mathrm{OLH}_2(4s+3,4)$ design, where $s \geq 5$ is an odd integer.

Case 2: $s \geq 4$ even: For $s = 4$, we have an $\mathrm{OLH}_2(19,4)$ obtained by deleting a column of the $\mathrm{OLH}_2(19,5)$ displayed in Table 2. Call this design $d_{19,4}$. Now, let $s \geq 6$. For $j = 1, 2, \ldots, (s-4)/2$, let E_j be an 8×4 matrix obtained by replacing the elements x_1, x_2, x_3 and x_4 by $10+4(j-1).11+4(j-1), 12+4(j-1)$ and $13+4(j-1)$, respectively, in the first orthogonal design of Table 1. Let

$$d^{(2)} = \begin{bmatrix} d_{19,4} \\ E_1 \\ E_2 \\ \vdots \\ E_{\frac{s-4}{2}} \end{bmatrix}.$$

Then, it is easily seen that $d^{(2)}$ is an $\mathrm{OLH}_2(4s+3,4)$ design, where $s \geq 6$ is an even integer.

In a special case, we can obtain an $\mathrm{OLH}_2(n,m)$ design with $m = 5$ columns. Suppose $n = 4s+3$ and $s \equiv 0 \pmod 4$. This implies that $n \equiv 3 \pmod{16}$. For $s = 4$, we have an $\mathrm{OLH}_2(19,5)$ design, displayed in Table 2. We denote this design by $d_{19,5}$. Let $s \equiv 0 \pmod 4$, $s \geq 8$. For $j = 1, 2, \ldots, (s-4)/4$, replace the elements $x_1, x_2, \ldots, x_8$ in any 5 columns of the second orthogonal design in Table 1 by $10+4(j-1), 11+4(j-1), \ldots, 17+4(j-1)$, respectively, to obtain the 16×5 matrices F_j, $j = 1, 2, \ldots, \frac{s-4}{4}$. Let

$d^{(3)}$ be the design

$$d^{(3)} = \begin{bmatrix} d_{19,5} \\ F_1 \\ F_2 \\ \vdots \\ F_{\frac{s-4}{4}} \end{bmatrix}.$$

Then $d^{(3)}$ is an $\mathrm{OLH}_2(4s+3,5)$ design where $s \equiv 0 \pmod 4$. We thus have the following result.

THEOREM 2. *Let* $n = 4s + 3$, *where* $s \equiv 0 \pmod 4$. *Then there exists an* $\mathrm{OLH}_2(4s+3,5)$ *design.*

TABLE 1
Orthogonal designs for $s = 4, 8$

$s = 4$

$$\begin{array}{rrrr}
x_1 & -x_2 & x_4 & x_3 \\
x_2 & x_1 & x_3 & -x_4 \\
x_3 & -x_4 & -x_2 & -x_1 \\
x_4 & x_3 & -x_1 & x_2 \\
-x_1 & x_2 & -x_4 & -x_3 \\
-x_2 & -x_1 & -x_3 & x_4 \\
-x_3 & x_4 & x_2 & x_1 \\
-x_4 & -x_3 & x_1 & -x_2
\end{array}$$

$s = 8$

$$\begin{array}{rrrrrrrr}
x_1 & -x_2 & -x_4 & -x_3 & -x_8 & x_7 & x_5 & x_6 \\
x_2 & x_1 & -x_3 & x_4 & -x_7 & -x_8 & -x_6 & x_5 \\
x_3 & -x_4 & x_2 & x_1 & -x_6 & -x_5 & x_7 & -x_8 \\
x_4 & x_3 & x_1 & -x_2 & -x_5 & x_6 & -x_8 & -x_7 \\
x_5 & -x_6 & -x_8 & x_7 & x_4 & x_3 & -x_1 & -x_2 \\
x_6 & x_5 & -x_7 & -x_8 & x_3 & -x_4 & x_2 & -x_1 \\
x_7 & -x_8 & x_6 & -x_5 & x_2 & -x_1 & -x_3 & x_4 \\
x_8 & x_7 & x_5 & x_6 & x_1 & x_2 & x_4 & x_3 \\
-x_1 & x_2 & x_4 & x_3 & x_8 & -x_7 & -x_5 & -x_6 \\
-x_2 & -x_1 & x_3 & -x_4 & x_7 & x_8 & x_6 & -x_5 \\
-x_3 & x_4 & -x_2 & -x_1 & x_6 & x_5 & -x_7 & x_8 \\
-x_4 & -x_3 & -x_1 & x_2 & x_5 & -x_6 & x_8 & x_7 \\
-x_5 & x_6 & x_8 & -x_7 & -x_4 & -x_3 & x_1 & x_2 \\
-x_6 & -x_5 & x_7 & x_8 & -x_3 & x_4 & -x_2 & x_1 \\
-x_7 & x_8 & -x_6 & x_5 & -x_2 & x_1 & x_3 & -x_4 \\
-x_8 & -x_7 & -x_5 & -x_6 & -x_1 & -x_2 & -x_4 & -x_3
\end{array}$$

Table 2

Orthogonal Latin hypercube designs $\mathrm{OLH}_{(}15,4)$ *and* $\mathrm{OLH}_{(}19,5)$

$\mathrm{OLH}_2(15,4)$

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

$\mathrm{OLH}_2(19,5)$

−9	8	1	1	8
−8	−3	7	6	−5
−7	4	−9	−8	−7
−6	−7	−4	7	−3
−5	1	5	−4	4
−4	−2	−6	3	2
−3	−6	3	−5	6
−2	−9	2	−9	−1
−1	5	8	−2	−9
0	0	0	0	0
9	−8	−1	−1	−8
8	3	−7	−6	5
7	−4	9	8	7
6	7	4	−7	3
5	−1	−5	4	−4
4	2	6	−3	−2
3	6	−3	5	−6
2	9	−2	9	1
1	−5	−8	2	9

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