CONSTRUCTION OF NESTED ORTHOGONAL LATIN HYPERCUBE DESIGNS

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Abstract: Nested Latin hypercube designs (LHDs) are proposed for conducting multiple computer experiments with different levels of accuracy. Orthogonality is shown to be an important feature. Little is known about the construction of nested orthogonal LHDs. We present methods to construct them with two or more layers, making use of orthogonal designs. The constructed designs possess the property that the sum of the elementwise products of any three columns is zero, which is shown to be desirable for factor screening.

Key words and phrases: Computer experiment, nested Latin hypercube design, orthogonal design, orthogonality.

1. Introduction

Latin hypercube designs (LHDs), introduced by McKay, Beckman, and Conover (1979), are widely used in computer experiments. An LHD with n runs and m factors is denoted by a matrix $L(n, m) = (l_1, \ldots, l_m)$, where l_j is the jth factor, and each factor includes n uniformly spaced levels. An LHD is called orthogonal if the correlation coefficient between any two columns of this LHD is zero.

A recent trend in sciences and engineering is to use both accurate (but slow) computer experiments and less accurate (but fast) computer experiments to study complex physical systems (see, for example, Qian et al. (2006)). In some cases, a large and expensive computer code can be executed at various degrees of fidelity, and result in computer experiments with multiple levels of cost and accuracy. Efficient data collection from these experiments is critical. Nested designs, proposed by Qian and Wu (2008), are useful for designing such experiments. Qian, Ai, and Wu (2009) and Qian, Tang, and Wu (2009) applied projections in Galois fields to obtain nested space-filling designs, that only exist for certain parameter values. Haaland and Qian (2010) constructed nested space-filling designs for multi-fidelity computer experiments based on (t, s)-sequences. Recently, Sun, Yin, and Liu (2013) presented a general approach to constructing nested space-filling designs using nested difference matrices. These nested space-filling designs

can achieve uniformity in low dimensions, but they lack orthogonality. The uniformity in two-dimensional projection implies that in any two dimensions, each of the $k \times k$ square bins contains the same number of points (the value of k depends on the number of the design points). There is no one-to-one relationship between uniformity and orthogonality, uniformity does not guarantee the orthogonality between any two columns, and vise versa. Li and Qian (2013) proposed (nearly) column-orthogonal LHDs for two-fidelity computer experiments.

In this paper, we propose a new class of nested orthogonal LHDs designated for multi-fidelity. These are useful for sequential experimentation, model building, model calibration, and validation in computer experiments. They can also be used for optimization under uncertainty methods, multi-level function estimation, linking parameters, and sequential evaluations (see, for example, Haaland and Qian (2010)). In addition, the resulting nested LHDs possess the property that the sum of the elementwise products of any three columns is zero.

The paper is organized as follows. In Section 2, we propose the method to construct nested orthogonal LHDs with two layers. The construction with three or more layers is developed in Section 3. Further results on the design properties and existence of these nested orthogonal LHDs are provided in Section 4. All proofs of theorems are in the Appendix.

2. Construction of Nested Orthogonal LHDs with Two Layers

This section discusses the construction of nested orthogonal LHDs with two layers. The construction is made possible by a special type of orthogonal design (OD) proposed by Yang and Liu (2012), as defined below.

Definition 1. An $m \times m$ matrix D is called an m-order OD with entries from $\pm(ia + b)$ for $i = 1, \ldots, m$ and $a \neq 0$, denoted by $OD(m)$, if it satisfies

(i) by changing $-(ia + b)$ to $ia + b$ (for $i = 1, \ldots, m$) in D, each column is a permutation of $\{ia + b, i = 1, \ldots, m\}$, and

(ii) the inner product of any two distinct columns is zero.

Note that $OD(m)$'s are available in Yang and Liu (2012) for $m = 2^r$, where r is any positive integer.

Consider a computer experiment involving u levels of accuracy: $Y_1(\cdot), \ldots, Y_u(\cdot)$, where $Y_u(\cdot)$ is the most accurate, $Y_{u-1}(\cdot)$ is the second most accurate, and so on. For each $i = 1, \ldots, u$, let L_i be the design associated with $Y_i(\cdot)$ consisting of n_i points. If the ith layer L_i is an $L(n_i, m)$ for $i = 1, \ldots, u$ with $L_u \subset \cdots \subset L_1$ and $n_u < \cdots < n_1$, then $(L_1; \ldots; L_u)$ is called a nested LHD with u layers. Furthermore, if each L_i is an orthogonal LHD, then $(L_1; \ldots; L_u)$ is called a nested orthogonal LHD, denoted $NOL((n_1, \ldots, n_u), m)$.

Theorem 1. *Suppose D is an $OD(m)$ with entries from $\pm(ia + b)$ for $i = 1, \ldots, m$, where $a \geq 2$ is an even integer. Let D_j be the corresponding design with $b = j - a$ for $j = 1, \ldots, a$,*

$$
\begin{aligned}
L_1 &= (D_1^T, \ldots, D_a^T, 0_m, -D_1^T, \ldots, -D_a^T)^T, \\
L_{2\alpha} &= (D_{a/2}^T, -D_{a/2}^T)^T, \quad L_{2\beta} = (D_a^T, 0_m, -D_a^T)^T, \\
L_{2\alpha}^* &= (D_1^T, -D_1^T, D_3^T, -D_3^T, \ldots, D_{a-1}^T, -D_{a-1}^T)^T, \\
L_{2\beta}^* &= (D_2^T, -D_2^T, D_4^T, -D_4^T, \ldots, D_a^T, 0_m, -D_a^T)^T,
\end{aligned}
\tag{2.1}
$$

where 0_m denotes the $m \times 1$ column vector with all elements zero. Then

(i) $(L_1; L_{2\alpha})$ *is an $NOL((2am + 1, 2m), m)$;*

(ii) $(L_1; L_{2\beta})$ *is an $NOL((2am + 1, 2m + 1), m)$;*

(iii) $(L_1; L_{2\alpha}^*)$ *is an $NOL((2am + 1, am), m)$, for $a > 2$;*

(iv) $(L_1; L_{2\beta}^*)$ *is an $NOL((2am + 1, am + 1), m)$, for $a > 2$.*

Example 1. Consider the $OD(4)$ matrix

$$
D = \begin{pmatrix}
a + b & 2a + b & -4a - b & 3a + b \\
2a + b & -a - b & -3a - b & -4a - b \\
3a + b & 4a + b & 2a + b & -a - b \\
4a + b & -3a - b & a + b & 2a + b
\end{pmatrix}.
$$

With $a = 4$, we get $D_1, D_2, D_3,$ and D_4 with $b = -3, -2, -1,$ and 0, respectively. Let

$$
\begin{aligned}
L_1 &= (D_2^T, -D_2^T, D_4^T, 0_4, -D_4^T, D_1^T, -D_1^T, D_3^T, -D_3^T)^T, \\
L_{2\alpha} &= (D_2^T, -D_2^T)^T, \qquad\qquad L_{2\beta} = (D_4^T, 0_4, -D_4^T)^T, \\
L_{2\alpha}^* &= (D_1^T, -D_1^T, D_3^T, -D_3^T)^T, \quad L_{2\beta}^* = (D_2^T, -D_2^T, D_4^T, 0_4, -D_4^T)^T.
\end{aligned}
$$

It can be easily verified that $(L_1; L_{2\alpha})$ is an $NOL((33, 8), 4)$, $(L_1; L_{2\beta})$ is an $NOL((33, 9), 4)$, $(L_1; L_{2\alpha}^*)$ is an $NOL((33, 16), 4)$ and $(L_1; L_{2\beta}^*)$ is an $NOL((33, 17), 4)$, as given in Table 1. Such nested orthogonal LHDs are apparently new and not available through any existing method. The design in Theorem 1 (ii) also works for odd a. As a special case of Theorem 1, if b only takes the values of 0 and $-a/2$, a special nested orthogonal LHD can be obtained, with two subarrays both orthogonal LHDs.

3. Construction of Nested Orthogonal LHDs with Three or More Layers

A method for constructing nested orthogonal LHDs with three layers is proposed here, followed by the construction of nested orthogonal LHDs with k $(k > 3)$ layers.

Table 1. An $NOL((33,8),4)$, $NOL((33,9),4)$, $NOL((33,16),4)$ or $NOL((33,17),4)$ from Example 1.

Run #	x_1	x_2	x_3	x_4	Run #	x_1	x_2	x_3	x_4
1	2	6	−14	10	18	1	5	−13	9
2	6	−2	−10	−14	19	5	−1	−9	−13
3	10	14	6	−2	20	9	13	5	−1
4	14	−10	2	6	21	13	−9	1	5
5	−2	−6	14	−10	22	−1	−5	13	−9
6	−6	2	10	14	23	−5	1	9	13
7	−10	−14	−6	2	24	−9	−13	−5	1
8	−14	10	−2	−6	25	−13	9	−1	−5
9	4	8	−16	12	26	3	7	−15	11
10	8	−4	−12	−16	27	7	−3	−11	−15
11	12	16	8	−4	28	11	15	7	−3
12	16	−12	4	8	29	15	−11	3	7
13	0	0	0	0	30	−3	−7	15	−11
14	−4	−8	16	−12	31	−7	3	11	15
15	−8	4	12	16	32	−11	−15	−7	3
16	−12	−16	−8	4	33	−15	11	−3	−7
17	−16	12	−4	−8					

Note: The entire array is an $L(33, 4)$, L_1; the subarray above the dashed line is an $L(8, 4)$, $L_{2\alpha}$; the subarray from Run 9 to Run 17 is an $L(9, 4)$, $L_{2\beta}$; the subarray from Run 1 to Run 17 is an $L(17, 4)$, $L_{2\beta}^*$; and the subarray from Run 18 to Run 33 is an $L(16, 4)$, $L_{2\alpha}^*$.

Theorem 2. *For the design L_1, $L_{2\alpha}^*$, and $L_{2\beta}^*$ of Theorem 1, let*

$$L_2 = (D_{a/2}^T, D_a^T, 0_m, -D_{a/2}^T, -D_a^T)^T,$$
$$L_{3\alpha} = (D_{a/2}^T, -D_{a/2}^T)^T, \text{ and } L_{3\beta} = (D_a^T, 0_m, -D_a^T)^T.$$

If $a \geq 2$ is an integer, then

(i) $(L_2; L_{3\alpha})$ *is an* $NOL((4m+1, 2m), m)$;

(ii) $(L_2; L_{3\beta})$ *is an* $NOL((4m+1, 2m+1), m)$.

If $a \geq 4$ and a is even, then

(i) $(L_1; L_2; L_{3\alpha})$ *is an* $NOL((2am+1, 4m+1, 2m), m)$;

(ii) $(L_1; L_2; L_{3\beta})$ *is an* $NOL((2am+1, 4m+1, 2m+1), m)$;

(iii) $(L_1; L_{2\beta}^*; L_{3\beta})$ *is an* $NOL((2am+1, am+1, 2m+1), m)$;

(iv) *if $a/2$ is even,* $(L_1; L_{2\beta}^*; L_{3\alpha})$ *is an* $NOL((2am+1, am+1, 2m), m)$; *otherwise,*

(v) $(L_1; L_{2\alpha}^*; L_{3\alpha})$ *is an* $NOL((2am+1, am, 2m), m)$.

Example 2. Consider the L_1 of Example 1, and let

$$L_{3\alpha} = \begin{pmatrix} D_2 \\ -D_2 \end{pmatrix} = \begin{pmatrix} 2 & 6 & -14 & 10 \\ 6 & -2 & -10 & -14 \\ 10 & 14 & 6 & -2 \\ 14 & -10 & 2 & 6 \\ -2 & -6 & 14 & -10 \\ -6 & 2 & 10 & 14 \\ -10 & -14 & -6 & 2 \\ -14 & 10 & -2 & -6 \end{pmatrix},$$

$$L_{3\beta} = \begin{pmatrix} D_4 \\ 0_4^T \\ -D_4 \end{pmatrix} = \begin{pmatrix} 4 & 8 & -16 & 12 \\ 8 & -4 & -12 & -16 \\ 12 & 16 & 8 & -4 \\ 16 & -12 & 4 & 8 \\ 0 & 0 & 0 & 0 \\ -4 & -8 & 16 & -12 \\ -8 & 4 & 12 & 16 \\ -12 & -16 & -8 & 4 \\ -16 & 12 & -4 & -8 \end{pmatrix},$$

and $L_2 = (L_{3\alpha}^T, L_{3\beta}^T)^T$, for $a = 4$, $L_2 = L_{2\beta}^*$. Then it can be shown that $(L_1; L_2; L_{3\alpha})$ is an $NOL((33, 17, 8), 4)$, and $(L_1; L_2; L_{3\beta})$ is an $NOL((33, 17, 9), 4)$.

The next theorem provides a general method for constructing nested orthogonal LHDs with more than three layers.

Theorem 3. *Let $a_1, a_2, \ldots, a_p(= a)$ be positive integers such that $a_i < a_{i+1}$ and $a_i | a_{i+1}$ for $i = 1, \ldots, p-1$, and let*

$$L_i = (D_{a_i}^T, D_{2a_i}^T, \ldots, D_a^T, 0_m, -D_{a_i}^T, -D_{2a_i}^T, \ldots, -D_a^T)^T, \quad i = 1, \ldots, p.$$

Then

(i) *$(L_1; L_2; \ldots; L_p)$ is a p-layer $NOL((2m(a/a_1) + 1, 2m(a/a_2) + 1, \ldots, 2m + 1), m)$;*

(ii) *if a/a_{p-1} is even, and $L_p^* = (D_{a/2}^T, -D_{a/2}^T)^T$, $(L_1; L_2; \ldots; L_p^*)$ is a p-layer $NOL((2m(a/a_1) + 1, 2m(a/a_2) + 1, \ldots, 2m), m)$.*

Example 3. Return to the $OD(4)$ in Example 1 for illustration. Take $a_1 = 1, a_2 = 2, a_3 = 4, a_4 = a = 8$, to obtain eight ODs with $b = -7, -6, \ldots, 0,$

Table 2. The nested orthogonal LHD with 4 layers in Example 3.

Run#	x_1	x_2	x_3	x_4	Run#	x_1	x_2	x_3	x_4	Run#	x_1	x_2	x_3	x_4
1	4	12	−28	20	23	−10	2	18	26	45	27	−19	3	11
2	12	−4	−20	−28	24	−18	−26	−10	2	46	−3	−11	27	−19
3	20	28	12	−4	25	−26	18	−2	−10	47	−11	3	19	27
4	28	−20	4	12	26	6	14	−30	22	48	−19	−27	−11	3
5	−4	−12	28	−20	27	14	−6	−22	−30	49	−27	19	−3	−11
6	−12	4	20	28	28	22	30	14	−6	50	5	13	−29	21
7	−20	−28	−12	4	29	30	−22	6	14	51	13	−5	−21	−29
8	−28	20	−4	−12	30	−6	−14	30	−22	52	21	29	13	−5
9	8	16	−32	24	31	−14	6	22	30	53	29	−21	5	13
10	16	−8	−24	−32	32	−22	−30	−14	6	54	−5	−13	29	−21
11	24	32	16	−8	33	−30	22	−6	−14	55	−13	5	21	29
12	32	−24	8	16	34	1	9	−25	17	56	−21	−29	−13	5
13	0	0	0	0	35	9	−1	−17	−25	57	−29	21	−5	−13
14	−8	−16	32	−24	36	17	25	9	−1	58	7	15	−31	23
15	−16	8	24	32	37	25	−17	1	9	59	15	−7	−23	−31
16	−24	−32	−16	8	38	−1	−9	25	−17	60	23	31	15	−7
17	−32	24	−8	−16	39	−9	1	17	25	61	31	−23	7	15
18	2	10	−26	18	40	−17	−25	−9	1	62	−7	−15	31	−23
19	10	−2	−18	−26	41	−25	17	−1	−9	63	−15	7	23	31
20	18	26	10	−2	42	3	11	−27	19	64	−23	−31	−15	7
21	26	−18	2	10	43	11	−3	−19	−27	65	−31	23	−7	−15
22	−2	−10	26	−18	44	19	27	11	−3					

Note: The subarray from Run 1 to Run 8 is an $L(8,4)$, L_4^*; the subarray from Run 9 to Run 17 is an $L(9,4)$, L_4; the subarray from Run 1 to Run 17 is an $L(17,4)$, L_3; the subarray from Run 1 to Run 33 is an $L(33,4)$, L_2; the entire array from Run 1 to Run 65 is an $L(65,4)$, L_1, a 4-layer nested orthogonal LHD.

respectively. Then

$L_1 = (D_1^T, \ldots, D_8^T, 0_4, -D_1^T, \ldots, -D_8^T)^T$ is an $L(65,4)$, as given in Table 2;

$L_2 = (D_4^T, -D_4^T, D_8^T, 0_4, -D_8^T, D_2^T, -D_2^T, D_6^T, -D_6^T)^T$ is an $L(33,4)$;

$L_3 = (D_4^T, -D_4^T, D_8^T, 0_4, -D_8^T)^T$ is an $L(17,4)$;

$L_4^* = (D_4^T, -D_4^T)^T$ is an $L(8,4)$, and $L_4 = (D_8^T, 0_4, -D_8^T)^T$ is an $L(9,4)$.

Obviously, all these L_i's are orthogonal and satisfy

$$L_4^* \subset L_3 \subset L_2 \subset L_1 \text{ and } L_4 \subset L_3 \subset L_2 \subset L_1.$$

Thus $(L_1; L_2; L_3; L_4^*)$ is a 4-layer $NOL((65, 33, 17, 8), 4)$, and $(L_1; L_2; L_3; L_4)$ is a 4-layer $NOL((65, 33, 17, 9), 4)$.

Table 3. Existence of $NOL((n_1, \ldots, n_u), m)$'s with $m = 2^r$.

u	$(n_1, \ldots, n_u)$	a	Method
2	$(2am+1, 2m+1)$	≥ 2	Theorem 1
2	$(2am+1, 2m)$	≥ 2, even	Theorem 1
2	$(2am+1, am), (2am+1, am+1)$	> 2, even	Theorem 1
2	$(4m+1, 2m), (4m+1, 2m+1)$	≥ 2	Theorem 2
3	$(2am+1, 4m+1, 2m)$	≥ 4, even	Theorem 2
3	$(2am+1, 4m+1, 2m+1)$	≥ 4, even	Theorem 2
3	$(2am+1, am+1, 2m+1)$	≥ 4, even	Theorem 2
3	$(2am+1, am+1, 2m)$	≥ 4, $a/2$ is even	Theorem 2
3	$(2am+1, am, 2m)$	≥ 4, $a/2$ is odd	Theorem 2
p	$(2m(a/a_1)+1, 2m(a/a_2)+1, \ldots, 2m+1)$	$a_i < a_{i+1}, a_i \mid a_{i+1}, a_p = a$	Theorem 3
p	$(2m(a/a_1)+1, 2m(a/a_2)+1, \ldots, 2m)$	$a_i < a_{i+1}, a_i \mid a_{i+1},$ $a_p = a, a/a_{p-1}$ is even	Theorem 3

4. Further Results and Discussion

Combining fold-over structures and the nested LHDs above, we have the following.

Theorem 4. *For any of the nested orthogonal LHDs of Theorems 1, 2 or 3, each layer possesses the property that the sum of the elementwise products of any three columns is zero.*

Let X denote the model matrix for the first-order model of a design with n runs and m factors, including a column of ones for the intercept. Let X_{int} denote the $n \times m(m-1)/2$ matrix with all the possible bilinear interactions, and X_{quad} denote the $n \times m$ matrix with all the pure quadratic terms. The alias matrices for the first-order model associated with all the pure quadratic terms and the bilinear interactions are then given by $(X'X)^{-1}X'X_{\text{quad}}$ and $(X'X)^{-1}X'X_{\text{int}}$, respectively. A good design for estimating the main effects should guarantee that these alias matrices are small—ideally 0. It is easy to see that if the sum of the elementwise products of any three columns equals zero, then these two alias matrices are both zero matrices.

The newly constructed LHDs in Sections 2 and 3 have the nesting property as well as that orthogonality property, but with a flexible size of layers that is not available through any existing approach. $NOL((n_1, \ldots, n_u), m)$'s listed in Table 3 can be easily constructed by the corresponding method indicated in the last column. Note that m is a power of 2 (2^r) in this paper. For other m, $OD(m)$'s can be possibly constructed by using Latin squares and Hadamard matrices, or by rotating orthogonal arrays. This deserves further study.

Besides the orthogonality, our nested orthogonal LHD has the property that the sum of the elementwise products of any three columns is zero; this is desirable

when fitting the first-order model with second-order effects (the quadratic effects and bilinear interactions) present (cf., Sun, Liu, and Lin (2009, 2010)). Yang and Liu (2012)). Such an orthogonal LHD guarantees that the estimates of all linear effects are uncorrelated with each other and with that of all second-order effects.

Appendix: Proofs of Theorems

A.1. Proof of Theorem 1

From the definitions of $L_1, L_{2\alpha}, L_{2\beta}, L_{2\alpha}^*$, and $L_{2\beta}^*$ in (2.1), it is obvious that the nested structures $L_{2\alpha} \subset L_1$, $L_{2\beta} \subset L_1$, $L_{2\alpha}^* \subset L_1$, and $L_{2\beta}^* \subset L_1$ hold.

We show the one-dimensional uniformity of these designs. From the definition of D_j, the elements in each column of $(D_j^T, -D_j^T)^T$ are $\{\pm j, \pm(a + j), \ldots, \pm((m-1)a + j)\}$, $j = 1, \ldots, a$. Namely,

$\{0, \pm 1, \pm 2, \ldots, \pm ma\}$ in each column of L_1,

$\{\pm a/2, \pm 3a/2, \ldots, \pm(2m-1)a/2\}$ in each column of $L_{2\alpha}$,

$\{0, \pm a, \pm 2a, \ldots, \pm ma\}$ in each column of $L_{2\beta}$,

$\{\pm 1, \pm 3, \ldots, \pm(ma-1)\}$ in each column of $L_{2\alpha}^*$, and

$\{0, \pm 2, \pm 4, \ldots, \pm ma\}$ in each column of $L_{2\beta}^*$.

Obviously, these elements are equally spaced. Thus, $(L_1; L_{2\alpha})$, $(L_1; L_{2\beta})$, $(L_1; L_{2\alpha}^*)$, and $(L_1; L_{2\beta}^*)$ are nested LHDs.

We show the orthogonality of the LHDs. From the orthogonality of $OD(m)$ and the definition of D_j, $j = 1, \ldots, a$,

$$L_{2\alpha}^T L_{2\alpha} = \frac{ma^2(2m+1)(2m-1)}{6} I_m, \quad L_{2\beta}^T L_{2\beta} = \frac{ma^2(m+1)(2m+1)}{3} I_m,$$

$$L_{2\alpha}^{*T} L_{2\alpha}^* = \frac{m^2 a^2(ma+1)}{2} I_m, \qquad L_{2\beta}^{*T} L_{2\beta}^* = \frac{ma(ma+1)(ma+2)}{6} I_m, \text{ and}$$

$$L_1^T L_1 = \frac{ma(ma+1)(2ma+1)}{3} I_m,$$

where I_m is the identity matrix of order m. Thus we complete the proof.

A.2. Proofs of Theorems 2 and 3

From the definitions of L_1, $L_{2\alpha}^*$, $L_{2\beta}^*$ in Theorem 1, L_2, $L_{3\alpha}$, $L_{3\beta}$ in Theorem 2, and $L_1, \ldots, L_p$, L_p^* in Theorem 3, the nested structures can be easily observed. And from the elements in each column of $(D_j^T, -D_j^T)^T$, for $j = 1, \ldots, a$, the elements in each column of these designs can be listed, which are equally spaced, thus these designs are LHDs. The orthogonality of the LHDs can be deduced from the orthogonality of D_j's, similarly as we do in the proof of Theorem 1.

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