Statistica Sinica **26** (2016), 1249-1267
doi:http://dx.doi.org/10.5705/ss.2014.029

A NEW CLASS OF NESTED (NEARLY) ORTHOGONAL LATIN HYPERCUBE DESIGNS

Xue Yang[1,2], Jian-Feng Yang[2], Dennis K. J. Lin[3] and Min-Qian Liu[2]

[1] *Tianjin University of Finance and Economics,* [2] *Nankai University and* [3] *The Pennsylvania State University*

Abstract: Nested Latin hypercube designs are useful for computer experiments with multi-fidelity and orthogonality is a desirable property for them. In this paper, we provide methods for constructing nested Latin hypercube designs with (exact or near) orthogonality. The constructed designs have flexible numbers of runs and factors with the desirable property that the sum of the elementwise product of any three columns is zero. The construction algorithms are given with theoretical support. Some designs are tabulated for practical use.

Key words and phrases: Autocorrelation function, computer experiment, orthogonal design.

1. Introduction

Computer experiments are used to study complex systems and have received considerable attention. Latin hypercube designs (LHDs) for them, introduced by McKay, Beckman, and Conover (1979), are particularly popular. Experiments with various levels of accuracy or fidelity have been widely used in sciences and engineering. Thus high-accuracy experiments are more accurate but slower and low-accuracy experiments are less accurate but faster (see, Kennedy and O'Hagan (2000), Qian and Wu (2008)). It is appealing to use LHDs with two layers to design computer experiments with two levels of accuracy for increasing prediction accuracy with limited cost. Qian, Tang, and Wu (2009) and Qian, Ai, and Wu (2009) proposed nested space-filling designs for multi-fidelity experiments by applying projections in the Galois field, and other algebraic techniques. Haaland and Qian (2010) provided a construction method for nested space-filling designs of multi-layer with the help of (t, s)-sequences. Sun, Yin, and Liu (2013) constructed nested space-filling designs by using nested difference matrices. Sun, Liu, and Qian (2014) proposed methods for constructing several classes of nested space-filling designs based on a new group projection, and other algebraic techniques. Although these constructions can achieve stratification in low dimensions, they are not orthogonal.

An LHD is orthogonal if the correlation coefficient of any two columns is zero. For a first-order model, such a design guarantees independent estimates of linear effects. For a second-order model, however, designs with (a) each design column is orthogonal to all the others, and (b) the sum of elementwise product of any three columns is zero, ensure that estimates of all linear effects are uncorrelated with each other, and with all quadratic effects and bilinear interactions (cf., Ye (1998), Sun, Liu, and Lin (2009, 2010), Yang and Liu (2012)). If (a) cannot be satisfied, it can be relaxed to (a′) each column is nearly orthogonal to the others in the design. An LHD satisfying (a) and (b) is said to be a second-order orthogonal LHD, and an LHD with properties (a′) and (b) is said to be a nearly orthogonal LHD.

Li and Qian (2013) provided some approaches to constructing nested orthogonal LHDs using nested rotation matrices and nested factorial designs. Yang, Liu, and Lin (2014) presented methods for constructing nested orthogonal LHDs using a special type of orthogonal design proposed by Yang and Liu (2012). Their designs have properties (a) and (b) with 2^s factors and different layers, where s is a positive integer. For practical use, however, nested LHDs with (exact or near) orthogonality are needed, but largely unavailable.

This paper proposes a new class of nested LHDs with (exact or near) orthogonality by using vectors with zero periodic autocorrelation function (PAF) provided by Georgiou and Efthimiou (2014). These designs satisfy (a) and (b), or properties (a′) and (b), have flexible numbers of runs, and 2, 4, 8, 12, 16, 20, and 24 factors, some of which cannot be obtained from Yang, Liu, and Lin (2014).

The paper is organized as follows. Section 2 presents useful notation and definitions. Section 3 provides methods for constructing nested orthogonal LHDs using vectors with zero PAF. Section 4 proposes methods to construct nested nearly orthogonal LHDs. Section 5 extends the results of Sections 3 and 4 to nested orthogonal and nearly orthogonal LHDs with more layers and gives some concluding remarks. All proofs are deferred to Appendix A.

2. Preliminary Results

This section gives some notation and definitions. For vectors $u = (u_1, \ldots, u_n)^T$ and $v = (v_1, \ldots, v_n)^T$, we write $\bar{u}$ and $\bar{v}$ for their means, and ρ_{uv} for their correlation coefficient. Throughout, we use 0_m and 1_m to denote the $m \times 1$ column vectors with all entries zero and one, respectively, and use R_l to denote the anti-diagonal identity matrix of order l with one on the anti-diagonal and zero elsewhere. A circulant matrix is a square matrix $B = (b_{ij})$ of order n with first row $b_1 = (b_{1,0}, b_{1,1}, \ldots, b_{1,n-1})$ and every next row being generated by a circulant permutation of its previous row, $b_{ij} = b_{1,j-i+1}$, where $j-i+1$ is taken modulo n,

$i = 2, \dots, n$ and $j = 0, \dots, n-1$. Let $A = \{A_j : A_j = (a_{j0}, a_{j1}, \dots, a_{j(l-1)}), j = 1, \dots, r\}$ be a set of r vectors of length l. The *periodic autocorrelation function* (PAF) $P_A(s)$ is defined, reducing $i+s$ modulo l, as

$$P_A(s) = \sum_{j=1}^{r} \sum_{i=0}^{l-1} a_{ji} a_{j,i+s}, \quad s = 0, \dots, l-1.$$

The set of vectors A is said to have zero PAF if $P_A(s) = 0$, for all $s = 1, \dots, l-1$, and is said to have constant PAF if $P_A(s) = \gamma$, for all $s = 1, \dots, l-1$ for some integer number γ. Georgiou and Efthimiou (2014) provided an algorithm to search for sets of vectors with zero PAF. Some are listed in Appendix B. These vectors are used in Georgiou and Efthimiou (2014) for the construction of LHDs that satisfy (a) and (b). A design $L(n, m)$ with n runs and m factors is called an LHD if it corresponds to an $n \times m$ matrix $X = (x_1, \dots, x_m)$, where column x_j is the jth factor and each factor includes n uniformly spaced levels.

Consider a computer experiment involving u different levels of accuracy: $Y_1(\cdot), \dots, Y_u(\cdot)$, where $Y_u(\cdot)$ is the most accurate, $Y_{u-1}(\cdot)$ is the second most accurate, and so on. For each $i = 1, \dots, u$, let L_i be a design with n_i points associated with $Y_i(\cdot)$. If the ith layer L_i is an $L(n_i, m)$ for $i = 1, \dots, u$ with $L_u \subset \cdots \subset L_1$ and $n_u < \cdots < n_1$, then $(L_1; \dots; L_u)$ is called a nested LHD with u layers, denoted by $NL((n_1, \dots, n_u), m)$ (cf., Yang, Liu, and Lin (2014)). If each L_i is an orthogonal LHD, then $(L_1; \dots; L_u)$ is called a nested orthogonal LHD; if L_1 is a nearly orthogonal LHD and each $L_i, i = 2, \dots, u$, is an orthogonal or nearly orthogonal LHD, then $(L_1; \dots; L_u)$ is called a nested nearly orthogonal LHD.

We provide methods to construct orthogonal matrices that are useful for the construction of nested LHDs with (exact or near) orthogonality.

Lemma 1 (Thm. 4.49 of Geramita and Seberry (1979)). *Suppose there exist circulant matrices B_1, B_2, B_3, B_4 of order l satisfying*

$$B_1 B_1^T + B_2 B_2^T + B_3 B_3^T + B_4 B_4^T = cI_l,$$

where c is a constant. Then the Goethal-Seidel array

$$GS = GS(B_1, B_2, B_3, B_4) = \begin{pmatrix} B_1 & B_2 R_l & B_3 R_l & B_4 R_l \\ -B_2 R_l & B_1 & -B_4^T R_l & B_3^T R_l \\ -B_3 R_l & B_4^T R_l & B_1 & -B_2^T R_l \\ -B_4 R_l & -B_3^T R_l & B_2^T R_l & B_1 \end{pmatrix}$$

is an orthogonal matrix of order $4l$.

Corollary 1. *If there are vectors B_1, B_2, B_3, B_4 of length l with zero PAF, they can be used as the first rows of circulant matrices in the Goethals-Seidel array to generate an orthogonal matrix of order $4l$.*

Following Kharaghani (2000), a set of square real matrices $\{B_1, B_2, \ldots, B_{2k}\}$ is said to be amicable if

$$\sum_{i=1}^{k}(B_{2i-1}B_{2i}^T - B_{2i}B_{2i-1}^T) = 0.$$

Lemma 2 (Thm. 1 of Kharaghani (2000)). *Let $\{B_1, B_2, \ldots, B_8\}$ be an amicable set of circulant matrices of order l, satisfying $\sum_{i=1}^{8} B_iB_i^T = cI_l$. Then the Kharaghani array*

$$K = \begin{pmatrix} B_1 & B_2 & B_4R_l & B_3R_l & B_6R_l & B_5R_l & B_8R_l & B_7R_l \\ -B_2 & B_1 & B_3R_l & -B_4R_l & B_5R_l & -B_6R_l & B_7R_l & -B_8R_l \\ -B_4R_l & -B_3R_l & B_1 & B_2 & -B_8^TR_l & B_7^TR_l & B_6^TR_l & -B_5^TR_l \\ -B_3R_l & B_4R_l & -B_2 & B_1 & B_7^TR_l & B_8^TR_l & -B_5^TR_l & -B_6^TR_l \\ -B_6R_l & -B_5R_l & B_8^TR_l & -B_7^TR_l & B_1 & B_2 & -B_4^TR_l & B_3^TR_l \\ -B_5R_l & B_6R_l & -B_7^TR_l & -B_8^TR_l & -B_2 & B_1 & B_3^TR_l & B_4^TR_l \\ -B_8R_l & -B_7R_l & -B_6^TR_l & B_5^TR_l & B_4^TR_l & -B_3^TR_l & B_1 & B_2 \\ -B_7R_l & B_8R_l & B_5^TR_l & B_6^TR_l & -B_3^TR_l & -B_4^TR_l & -B_2 & B_1 \end{pmatrix}$$

is an orthogonal matrix of order $8l$.

Remark 1. As in Corollary 1, we can use eight vectors of length l with zero PAF to generate eight suitable amicable circulant matrices for Lemma 2.

Lemma 3. *Suppose there exist two circulant matrices B_1, B_2 of order l satisfying $B_1B_1^T + B_2B_2^T = cI_l$. Then*

$$B = \begin{pmatrix} B_1 & B_2 \\ -B_2^T & B_1^T \end{pmatrix} \quad or \quad B = \begin{pmatrix} B_1 & B_2R_l \\ -B_2R_l & B_1 \end{pmatrix} \tag{2.1}$$

is an orthogonal matrix of order $2l$.

Remark 2. Two vectors of length l with zero PAF can be used as the first rows of the circulant matrices B_1 and B_2 at (2.1) to generate an orthogonal matrix of order $2l$.

3. Generation of Nested Orthogonal LHDs

Here we construct nested orthogonal LHDs by using a special class of orthogonal matrices with order $2l$, $4l$, and $8l$. The generated designs have flexible run sizes and satisfy properties (a) and (b).

Two algorithms are provided to construct nested orthogonal LHDs with $m = rl$ factors. Given a positive integer a, let $A_1^b, A_2^b, \ldots, A_r^b$ be row vectors of length l with zero PAF and satisfying one of

(i) the set formed by combining the absolute values of all entries of all vectors together is $\{b+(2p-1)a : p=1,\ldots,m\}$;

(ii) the set formed by combining the absolute values of all entries of all vectors together is $\{b+pa : p=1,\ldots,m\}$.

Some vectors with zero PAF are listed in Appendix B, which were obtained by the algorithm provided in Georgiou and Efthimiou (2014). If the vectors satisfy (i), NOL-Algorithm 1 is used; if the vectors satisfy (ii), NOL-Algorithm 2 is used. The nested orthogonal LHDs generated by the two algorithms may have the same run size and number of factors. For ease of expression, we henceforth use r to denote $2, 4$, or 8, and use $D_{i\pm j}$ to denote the matrices D_{i+j} and D_{i-j}.

Nested orthogonal LHDs Algorithm 1 (NOL-Algorithm 1)**.**

Step 1. Given a positive integer a, take $A_1^b, A_2^b, \ldots, A_r^b$ to be r row vectors of length l with zero PAF satisfying Condition (i).

Step 2. For $b=0,\pm1,\ldots,\pm(a-1),a$, construct E by stacking $D_0, D_{\pm1},\ldots, D_{\pm(a-1)}, D_a$ row by row, $E=(D_0^T, D_{\pm1}^T,\ldots,D_{\pm(a-1)}^T, D_a^T)^T$. Define $L_1=(-E^T, 0_m, E^T)^T$, $L_{2\alpha}=(-D_0^T, D_0^T)^T$, and $L_{2\beta}=(-D_a^T, 0_m, D_a^T)^T$.

Step 3. Let $F_1=(L_1; L_{2\alpha})$ and $F_2=(L_1; L_{2\beta})$.

Nested orthogonal LHDs Algorithm 2 (NOL-Algorithm 2)**.**

Step 1. Given a positive even integer a, take $A_1^b, A_2^b, \ldots, A_r^b$ to be r row vectors of length l with zero PAF satisfying Condition (ii).

Step 2. For $b=0,-1,\ldots,-(a-1)$, construct E by stacking $D_0, D_{-1},\ldots,D_{-(a-1)}$ row by row, $E=(D_0^T, D_{-1}^T,\ldots,D_{-(a-1)}^T)^T$. Define $L_1=(-E^T, 0_m, E^T)^T$, $L_{2\alpha}=(-D_0^T, 0_m, D_0^T)^T$, and $L_{2\beta}=(-D_{-a/2}^T, D_{-a/2}^T)^T$.

Step 3. Let $G_1=(L_1; L_{2\alpha})$ and $G_2=(L_1; L_{2\beta})$.

Theorem 1.

(i) *For the designs constructed in NOL-Algorithm 1, F_1 is a nested orthogonal $L((4am+1, 2m), m)$ and F_2 is a nested orthogonal $L((4am+1, 2m+1), m)$, where L_1, $L_{2\alpha}$, and $L_{2\beta}$ are orthogonal LHDs with m factors and $4am+1$, $2m$, and $2m+1$ runs, respectively.*

(ii) *For the designs constructed in NOL-Algorithm 2, G_1 is a nested orthogonal $L((2am+1, 2m+1), m)$ and G_2 is a nested orthogonal $L((2am+1, 2m), m)$, where L_1, $L_{2\alpha}$, and $L_{2\beta}$ are orthogonal LHDs with m factors and $2am+1$, $2m+1$, and $2m$ runs, respectively.*

Remark 3. NOL-Algorithm 2 works for any positive integer a. The condition that a be a positive even integer is to ensure that all levels of the generated designs are integers. NOL-Algorithms-1 and -2 are able to generate many new nested orthogonal LHDs that are not now available.

The following examples show how to construct designs with $m = 12$ and 20 factors. They are apparently new.

Example 1 ($m = 12$)**.** We construct nested orthogonal $L((48a+1, 24), 12)$, $L((48a+1, 25), 12)$, $L((49, 24), 12)$, and $L((49, 25), 12)$. By setting $a = 2$ in NOL-Algorithm 1, we have $b = -1, 0, 1, 2$. Then, by Corollary 1, vectors with zero PAF (in Appendix B) are $A_1^b = (b+15a, -(b+5a), b+19a)$, $A_2^b = (b+17a, -(b+21a), b+23a)$, $A_3^b = (b+a, b+3a, -(b+7a))$, and $A_4^b = (b+9a, b+11a, b+13a)$, and orthogonal matrices D_{-1}, D_0, D_1, and D_2 of order 12 are

$$D_{-1} = \left(\begin{array}{rrr|rrr|rrr|rrr}
29 & -9 & 37 & 45 & -41 & 33 & -13 & 5 & 1 & 25 & 21 & 17 \\
37 & 29 & -9 & -41 & 33 & 45 & 5 & 1 & -13 & 21 & 17 & 25 \\
-9 & 37 & 29 & 33 & 45 & -41 & 1 & -13 & 5 & 17 & 25 & 21 \\
\hline
-45 & 41 & -33 & 29 & -9 & 37 & -21 & -25 & -17 & 5 & -13 & 1 \\
41 & -33 & -45 & 37 & 29 & -9 & -25 & -17 & -21 & -13 & 1 & 5 \\
-33 & -45 & 41 & -9 & 37 & 29 & -17 & -21 & -25 & 1 & 5 & -13 \\
\hline
13 & -5 & -1 & 21 & 25 & 17 & 29 & -9 & 37 & 41 & -45 & -33 \\
-5 & -1 & 13 & 25 & 17 & 21 & 37 & 29 & -9 & -45 & -33 & 41 \\
-1 & 13 & -5 & 17 & 21 & 25 & -9 & 37 & 29 & -33 & 41 & -45 \\
\hline
-25 & -21 & -17 & -5 & 13 & -1 & -41 & 45 & 33 & 29 & -9 & 37 \\
-21 & -17 & -25 & 13 & -1 & -5 & 45 & 33 & -41 & 37 & 29 & -9 \\
-17 & -25 & -21 & -1 & -5 & 13 & 33 & -41 & 45 & -9 & 37 & 29
\end{array}\right),$$

$$D_{0} = \left(\begin{array}{rrr|rrr|rrr|rrr}
30 & -10 & 38 & 46 & -42 & 34 & -14 & 6 & 2 & 26 & 22 & 18 \\
38 & 30 & -10 & -42 & 34 & 46 & 6 & 2 & -14 & 22 & 18 & 26 \\
-10 & 38 & 30 & 34 & 46 & -42 & 2 & -14 & 6 & 18 & 26 & 22 \\
\hline
-46 & 42 & -34 & 30 & -10 & 38 & -22 & -26 & -18 & 6 & -14 & 2 \\
42 & -34 & -46 & 38 & 30 & -10 & -26 & -18 & -22 & -14 & 2 & 6 \\
-34 & -46 & 42 & -10 & 38 & 30 & -18 & -22 & -26 & 2 & 6 & -14 \\
\hline
14 & -6 & -2 & 22 & 26 & 18 & 30 & -10 & 38 & 42 & -46 & -34 \\
-6 & -2 & 14 & 26 & 18 & 22 & 38 & 30 & -10 & -46 & -34 & 42 \\
-2 & 14 & -6 & 18 & 22 & 26 & -10 & 38 & 30 & -34 & 42 & -46 \\
\hline
-26 & -22 & -18 & -6 & 14 & -2 & -42 & 46 & 34 & 30 & -10 & 38 \\
-22 & -18 & -26 & 14 & -2 & -6 & 46 & 34 & -42 & 38 & 30 & -10 \\
-18 & -26 & -22 & 12 & -6 & 14 & 34 & -42 & 46 & -10 & 38 & 30
\end{array}\right),$$

$$D_{1} = \left(\begin{array}{rrr|rrr|rrr|rrr}
31 & -11 & 39 & 47 & -43 & 35 & -15 & 7 & 3 & 27 & 23 & 19 \\
39 & 31 & -11 & -43 & 35 & 47 & 7 & 3 & -15 & 23 & 19 & 27 \\
-11 & 39 & 31 & 35 & 47 & -43 & 3 & -15 & 7 & 19 & 27 & 23 \\
\hline
-47 & 43 & -35 & 31 & -11 & 39 & -23 & -27 & -19 & 7 & -15 & 3 \\
43 & -35 & -47 & 39 & 31 & -11 & -27 & -19 & -23 & -15 & 3 & 7 \\
-35 & -47 & 43 & -11 & 39 & 31 & -19 & -23 & -27 & 3 & 7 & -15 \\
\hline
15 & -7 & -3 & 23 & 27 & 19 & 31 & -11 & 39 & 43 & -47 & -35 \\
-7 & -3 & 15 & 27 & 19 & 23 & 39 & 31 & -11 & -47 & -35 & 43 \\
-3 & 15 & -7 & 19 & 23 & 27 & -11 & 39 & 31 & -35 & 43 & -47 \\
\hline
-27 & -23 & -19 & -7 & 15 & -3 & -43 & 47 & 35 & 31 & -11 & 39 \\
-23 & -19 & -27 & 15 & -3 & -7 & 47 & 35 & -43 & 39 & 31 & -11 \\
-19 & -27 & -23 & -3 & -7 & 15 & 35 & -43 & 47 & -11 & 39 & 31
\end{array}\right),$$

$$D_2 = \left(\begin{array}{rrr|rrr|rrr|rrr}
32 & -12 & 40 & 48 & -44 & 36 & -16 & 8 & 4 & 28 & 24 & 20 \\
40 & 32 & -12 & -44 & 36 & 48 & 8 & 4 & -16 & 24 & 20 & 28 \\
-12 & 40 & 32 & 36 & 48 & -44 & 4 & -16 & 8 & 20 & 28 & 24 \\
\hline
-48 & 44 & -36 & 32 & -12 & 40 & -24 & -28 & -20 & 8 & -16 & 4 \\
44 & -36 & -48 & 40 & 32 & -12 & -28 & -20 & -24 & -16 & 4 & 8 \\
-36 & -48 & 44 & -12 & 40 & 32 & -20 & -24 & -28 & 4 & 8 & -16 \\
\hline
16 & -8 & -4 & 24 & 28 & 20 & 32 & -12 & 40 & 44 & -48 & -36 \\
-8 & -4 & 16 & 28 & 20 & 24 & 40 & 32 & -12 & -48 & -36 & 44 \\
-4 & 16 & -8 & 20 & 24 & 28 & -12 & 40 & 32 & -36 & 44 & -48 \\
\hline
-28 & -24 & -20 & -8 & 16 & -4 & -44 & 48 & 36 & 32 & -12 & 40 \\
-24 & -20 & -28 & 16 & -4 & -8 & 48 & 36 & -44 & 40 & 32 & -12 \\
-20 & -28 & -24 & -4 & -8 & 16 & 36 & -44 & 48 & -12 & 40 & 32
\end{array}\right).$$

By NOL-Algorithm 1, $(L_1; L_{2\alpha})$ and $(L_1; L_{2\beta})$ are nested orthogonal $L((97,24),12)$ and $L((97,25),12)$, respectively, where

$L_1 = (-D_0^T, D_0^T, -D_2^T, 0_{12}, D_2^T, -D_{-1}^T, D_{-1}^T, -D_1^T, D_1^T,)^T$ is an orthogonal $L(97,12)$,

$L_{2\alpha} = (-D_0^T, D_0^T)^T$ is an orthogonal $L(24,12)$, and

$L_{2\beta} = (-D_2^T, 0_{12}, D_2^T)^T$ is an orthogonal $L(25,12)$.

Furthermore, by letting $L_1' = (L_{2\alpha}^T, L_{2\beta}^T)^T$, we have that $(L_1'; L_{2\alpha})$ and $(L_1'; L_{2\beta})$ are nested orthogonal $L((49,24),12)$ and $L((49,25),12)$, respectively. If we take other values for a, then more nested orthogonal LHDs with 12 factors and flexible run sizes can be constructed similarly.

Example 2 ($m = 20$)**.** We construct nested orthogonal LHDs with 20 factors. Set $a = 2$ in NOL-Algorithm 2, then $b = 0, -1$. Vectors with zero PAF (in Appendix B) are $A_1^b = (b + 11a, b + 3a, -(b + 14a), b + 15a, b + 12a)$, $A_2^b = (b+13a, b+16a, b+17a, b+18a, -(b+19a))$, $A_3^b = (b+20a, b+a, -(b+2a), -(b+4a), -(b+5a))$, and $A_4^b = (b+6a, b+7a, -(b+8a), b+9a, -(b+10a))$. According to Corollary 1 and NOL-Algorithm 2, nested orthogonal $L((81,41),20)$ and $L((81,40),20)$ can be obtained: $(L_1; L_{2\alpha})$ and $(L_1; L_{2\beta})$ with $L_1 = (L_{2\alpha}^T, L_{2\beta}^T)^T$, $L_{2\alpha} = (-D_0^T, 0_{20}, D_0^T)^T$, and $L_{2\beta} = (-D_{-1}^T, D_{-1}^T)^T$, where D_0 and D_{-1} are listed in Appendix C.

4. Generation of Nested Nearly Orthogonal LHDs

For some parameters, a nested LHD with orthogonality may not exist. Then a nested nearly orthogonal LHD is a natural choice. We propose two methods for constructing nested nearly orthogonal LHDs, that satisfy properties (a′) and (b) in Section 1, using r vectors with zero PAF. The main difference with the algorithms in Section 3 is that two more runs are added. To achieve a low correlation between any two distinct columns, levels $+1$ and -1 are added and original nonzero levels are taken further away from zero to make sure the resulting design is an LHD.

Nested nearly orthogonal LHDs Algorithm 1 (NNOL-Algorithm 1)**.**

Step 1. The same as Step 1 of NOL-Algorithm 1, except that here $a \geq 2$.

Step 2. For $b = 0, \pm 1, \ldots, \pm(a-2), a-1, a, a+1$, construct E by stacking $D_0, D_{\pm 1}, \ldots, D_{\pm(a-2)}, D_{a-1}, D_a, D_{a+1}$ row by row, $E = (D_0^T, D_{\pm 1}^T, \ldots, D_{\pm(a-2)}^T, D_{a-1}^T, D_a^T, D_{a+1}^T)^T$. Define $L_1 = (-E^T, -1_m, 0_m, 1_m, E^T)^T$.

Step 3. Let $Q_1 = (L_1; L_{2\alpha})$ and $Q_2 = (L_1; L_{2\beta})$, where $L_{2\alpha}$ and $L_{2\beta}$ have the same form as in NOL-Algorithm 1.

Nested nearly orthogonal LHDs Algorithm 2 (NNOL-Algorithm 2)**.**

Step 1. The same as Step 1 of NOL-Algorithm 2.

Step 2. For $b = 1, 0, -1, \ldots, -(a-2)$, construct E by stacking $D_1, D_0, D_{-1}, \ldots, D_{-(a-2)}$ row by row, $E = (D_1^T, D_0^T, D_{-1}^T, \ldots, D_{-(a-2)}^T)^T$. Define $L_1 = (-E^T, -1_m, 0_m, 1_m, E^T)^T$.

Step 3. Let $W_1 = (L_1; L_{2\alpha})$ and $W_2 = (L_1; L_{2\beta})$, where $L_{2\alpha}$ and $L_{2\beta}$ have the same form as in NOL-Algorithm 2.

Theorem 2.

(i) *For the designs constructed in NNOL-Algorithm* 1*,* Q_1 *is a nested nearly orthogonal* $L((4am+3, 2m), m)$ *and* Q_2 *is a nested nearly orthogonal* $L((4am+3, 2m+1), m)$*, where* L_1 *is a nearly orthogonal LHD with correlation* $\rho_{uv} = 6/[(2am+1)(2am+2)(4am+3)]$ *for any two distinct columns* u *and* v*,* $L_{2\alpha}$ *and* $L_{2\beta}$ *are orthogonal LHDs with* m *factors and* $2m$ *and* $2m+1$ *runs, respectively.*

(ii) *For the designs constructed in NNOL-Algorithm* 2*,* W_1 *is a nested nearly orthogonal* $L((2am+3, 2m+1), m)$ *and* W_2 *is a nested nearly orthogonal* $L((2am+3, 2m), m)$*, where* L_1 *is a nearly orthogonal LHD with correlation* $\rho_{uv} = 6/[(am+1)(am+2)(2am+3)]$ *for any two distinct columns* u *and* v*,* $L_{2\alpha}$ *and* $L_{2\beta}$ *are orthogonal LHDs with* m *factors and* $2m+1$ *and* $2m$ *runs, respectively.*

The W_1 in NNOL-Algorithm 2 also works for odd a with $a > 2$; an illustration is given in Example 5. The resulting design in Theorem 2 is not orthogonal, but the correlation between any two design columns is a small constant as given in Theorem 2. We thus call them nearly orthogonal.

Example 3 ($m = 8$)**.** We construct a nested nearly orthogonal $L((32a+3, 16), 8)$ and $L((32a+3, 17), 8)$ by using Lemma 2 and the eight vectors $A_i^b = b + (2i-1)a$ for $i = 1, \ldots, 8$ with zero PAF. Without loss of generality, take $a = 2$, and then

$b = 0, 1, 2, 3$ from NNOL-Algorithm 1. We get orthogonal matrices D_0, D_1, D_2, and D_3 of order eight as

$$D_0 = \begin{pmatrix} 2 & 6 & 14 & 10 & 22 & 18 & 30 & 26 \\ -6 & 2 & 10 & -14 & 18 & -20 & 26 & -30 \\ -14 & -10 & 2 & 6 & -30 & 26 & 22 & -18 \\ -10 & 14 & -6 & 2 & 26 & 30 & -18 & -22 \\ -22 & -18 & 30 & -26 & 2 & 6 & -14 & 10 \\ -18 & 22 & -26 & -30 & -6 & 2 & 10 & 14 \\ -30 & -26 & -22 & 18 & 14 & -10 & 2 & 6 \\ -26 & 30 & 18 & 22 & -10 & -14 & -6 & 2 \end{pmatrix},$$

$$D_1 = \begin{pmatrix} 3 & 7 & 15 & 11 & 23 & 19 & 31 & 27 \\ -7 & 3 & 11 & -15 & 19 & -21 & 27 & -31 \\ -15 & -11 & 3 & 7 & -31 & 27 & 23 & -19 \\ -11 & 15 & -7 & 3 & 27 & 31 & -19 & -23 \\ -23 & -19 & 31 & -27 & 3 & 7 & -15 & 11 \\ -19 & 23 & -27 & -31 & -7 & 3 & 11 & 15 \\ -31 & -27 & -23 & 19 & 15 & -11 & 3 & 7 \\ -27 & 31 & 19 & 23 & -11 & -15 & -7 & 3 \end{pmatrix},$$

$$D_2 = \begin{pmatrix} 4 & 8 & 16 & 12 & 24 & 20 & 32 & 28 \\ -8 & 4 & 12 & -16 & 20 & -22 & 28 & -32 \\ -16 & -12 & 4 & 8 & -32 & 28 & 24 & -20 \\ -12 & 16 & -8 & 4 & 28 & 32 & -20 & -24 \\ -24 & -20 & 32 & -28 & 4 & 8 & -16 & 12 \\ -20 & 24 & -28 & -32 & -8 & 4 & 12 & 16 \\ -32 & -28 & -24 & 20 & 16 & -12 & 4 & 8 \\ -28 & 32 & 20 & 24 & -12 & -16 & -8 & 4 \end{pmatrix},$$

$$D_3 = \begin{pmatrix} 5 & 9 & 17 & 13 & 25 & 21 & 33 & 29 \\ -9 & 5 & 13 & -17 & 21 & -23 & 29 & -33 \\ -17 & -13 & 5 & 9 & -33 & 29 & 25 & -21 \\ -13 & 17 & -9 & 5 & 29 & 33 & -21 & -25 \\ -25 & -21 & 33 & -29 & 5 & 9 & -17 & 13 \\ -21 & 25 & -29 & -33 & -9 & 5 & 13 & 17 \\ -33 & -29 & -25 & 21 & 17 & -13 & 5 & 9 \\ -29 & 33 & 21 & 25 & -13 & -17 & -9 & 5 \end{pmatrix}.$$

By using them, we obtain nested nearly orthogonal LHDs $(L_1; L_{2\alpha})$ and $(L_1; L_{2\beta})$ of 8 factors with correlation $\rho_{uv} = 1/12,529$, where $L_1 = (D_0^T, -D_0^T, D_2^T, -D_2^T, 0_8, D_1^T, -D_1^T, D_3^T, -D_3^T, 1_8, -1_8)^T$ is a nearly orthogonal $L(67, 8)$, $L_{2\alpha} = (D_0^T, -D_0^T)^T$ is an orthogonal $L(16, 8)$, and $L_{2\beta} = (D_2^T, -D_2^T, 0_8)^T$ is an orthogonal $L(17, 8)$.

Table 1. The nested nearly orthogonal LHD with 8 factors and 67 runs in Example 3.

Run	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	Run	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
1	2	6	14	10	22	18	30	26	34	3	7	15	11	23	19	31	27
2	−6	2	10	−14	18	−20	26	−30	35	−7	3	11	−15	19	−21	27	−31
3	−14	−10	2	6	−30	26	22	−18	36	−15	−11	3	7	−31	27	23	−19
4	−10	14	−6	2	26	30	−18	−22	37	−11	15	−7	3	27	31	−19	−23
5	−22	−18	30	−26	2	6	−14	10	38	−23	−19	31	−27	3	7	−15	11
6	−18	22	−26	−30	−6	2	10	14	39	−19	23	−27	−31	−7	3	11	15
7	−30	−26	−22	18	14	−10	2	6	40	−31	−27	−23	19	15	−11	3	7
8	−26	30	18	22	−10	−14	−6	2	41	−27	31	19	23	−11	−15	−7	3
9	−2	−6	−14	−10	−22	−18	−30	−26	42	−3	−7	−15	−11	−23	−19	−31	−27
10	6	−2	−10	14	−18	20	−26	30	43	7	−3	−11	15	−19	21	−27	31
11	14	10	−2	−6	30	−26	−22	18	44	15	11	−3	−7	−31	27	−23	19
12	10	−14	6	−2	−26	−30	18	22	45	11	−15	7	−3	−27	−31	19	23
13	22	18	−30	26	−2	−6	14	−10	46	23	19	−31	27	−3	−7	15	−11
14	18	−22	26	30	6	−2	−10	−14	47	19	−23	27	31	7	−3	−11	−15
15	30	26	22	−18	−14	10	−2	−6	48	31	27	23	−19	−15	11	−3	−7
16	26	−30	−18	−22	10	14	6	−2	49	27	−31	−19	−23	11	15	7	−3
17	4	8	16	12	24	20	32	28	50	5	9	17	13	25	21	33	29
18	−8	4	12	−16	20	−22	28	−32	51	−9	5	13	−17	21	−23	29	−33
19	−16	−12	4	8	−32	28	24	−20	52	−17	−13	5	9	−33	29	25	−21
20	−12	16	−8	4	28	32	−20	−24	53	−13	17	−9	5	29	33	−21	−25
21	−24	−20	32	−28	4	8	−16	12	54	−25	−21	33	−29	5	9	−17	13
22	−20	24	−28	−32	−8	4	12	16	55	−21	25	−29	−33	−9	5	13	17
23	−32	−28	−24	20	16	−12	4	8	56	−33	−29	−25	21	17	−13	5	9
24	−28	32	20	24	−12	−16	−8	4	57	−29	33	21	25	−13	−17	−9	5
25	−4	−8	−16	−12	−24	−20	−32	−28	58	−5	−9	−17	−13	−25	−21	−33	−29
26	8	−4	−12	16	−20	22	−28	32	59	9	−5	−13	17	−21	23	−29	33
27	16	12	−4	−8	32	−28	−24	20	60	17	13	−5	−9	33	−29	−25	21
28	12	−16	8	−4	−28	−32	20	24	61	13	−17	9	−5	−29	−33	21	25
29	24	20	−32	28	−4	−8	16	−12	62	25	21	−33	29	−5	−9	17	−13
30	20	−24	28	32	8	−4	−12	−16	63	21	−25	29	33	9	−5	−13	−17
31	32	28	24	−20	−16	12	−4	−8	64	33	29	25	−21	−17	13	−5	−9
32	28	−32	−20	−24	12	16	8	−4	65	29	−33	−21	−25	13	17	9	−5
33	0	0	0	0	0	0	0	0	66	1	1	1	1	1	1	1	1
									67	−1	−1	−1	−1	−1	−1	−1	−1

Note: The entire array is a nearly orthogonal $L(67,8)$ with correlation $\rho_{uv} = 1/12,529$, L_1; the subarray above the dashed line is an orthogonal $L(16,8)$, $L_{2\alpha}$; and the subarray from Run 17 to Run 33 is an orthogonal $L(17,8)$, $L_{2\beta}$.

The generated design $(L_1; L_{2\alpha})$ is a nested nearly orthogonal $L((67,16),8)$, and $(L_1; L_{2\beta})$ is a nested nearly orthogonal $L((67,17),8)$. These are given in Table 1.

5. Extensions and Concluding Remarks

Nested Latin hypercube designs (LHDs) are useful for sequentially running a computer model, validating a computer model, and solving stochastic optimization problems (Qian (2009)). We propose a new class of nested orthogonal and nearly orthogonal LHDs with two layers. Extensions can be made in two directions. First, if $a \geq 4$ is an even integer, it is easy to construct nested orthogonal and nested nearly orthogonal LHDs with multiple layers by extending our algorithms, as in the following example.

Example 4 ($m = 4$)**.** We construct nested nearly orthogonal LHDs with four layers. Take vectors $A_1 = b + a$, $A_2 = b + 3a$, $A_3 = b + 5a$, $A_4 = b + 7a$. For $a = 4$, and $b = 0, \pm 1, \pm 2, 3, 4, 5$, the eight corresponding orthogonal matrices are $D_0, D_{\pm 1}, D_{\pm 2}, D_3, D_4$, and D_5. We obtain 4-layer nested nearly orthogonal LHDs $(H; H_3; H_2; H_\alpha)$ and $(H; H_3; H_2; H_\beta)$ with 4 factors, where $H = (-D_0^T, D_0^T, -D_4^T, 0_4, D_4^T, -D_{-2}^T, D_{-2}^T, -D_2^T, D_2^T, -D_{-1}^T, D_{-1}^T, -D_1^T, D_1^T, -D_3^T, D_3^T, -D_5^T, D_5^T, 1_4, -1_4)^T$ is a nearly orthogonal $L(67, 4)$ with $\rho_{uv} = 1/12,529$; $H_3 = (-D_0^T, D_0^T, -D_4^T, 0_4, D_4^T, -D_{-2}^T, D_{-2}^T, -D_2^T, D_2^T)^T$ is an orthogonal $L(33, 4)$; $H_2 = (-D_0^T, D_0^T, -D_4^T, 0_4, D_4^T)^T$ is an orthogonal $L(17, 4)$; $H_\alpha = (-D_0^T,\ D_0^T)^T$ is an orthogonal $L(8, 4)$; and $H_\beta = (-D_4^T, 0_4,\ D_4^T)^T$ is an orthogonal $L(9, 4)$. The resulting design is displayed in Table 2.

As well, the run size of nested (nearly) orthogonal LHDs obtained from NOL-Algorithms and NNOL-Algorithms can be more flexible if the parameter b in vectors with zero PAF takes other values. We rewrite NNOL-Algorithm 2 to show such extension.

Nested nearly orthogonal LHDs Algorithm 3 (NNOL-Algorithm 2*)**.**
Step 1. The same as Step 1 of NOL-Algorithm 2.

Step 2. For $j = 0, \ldots, k-1$ with k being a positive integer, define $E_j = (D_{amj+1}^T, D_{amj}^T, D_{amj-1}^T, \ldots, D_{amj-(a-2)}^T)^T$ and $L_1 = (-E_{k-1}^T, \ldots, -E_0^T, -1_m, 0_m, 1_m, E_0^T, \ldots, E_{k-1}^T)^T$.

Step 3. Let $W_1 = (L_1; L_{2\alpha})$ and $W_2 = (L_1; L_{2\beta})$, where $L_{2\alpha}$ and $L_{2\beta}$ have the same form as in NOL-Algorithm 2.

Here W_1 is a nested nearly orthogonal $L((2amk+3, 2mk+1), m)$ and W_2 is a nested nearly orthogonal $L((2amk+3, 2mk), m)$, where L_1 is a nearly orthogonal LHD with correlation $\rho_{uv} = 6/[(amk+1)(amk+2)(2amk+3)]$ for any two distinct columns u and v, $L_{2\alpha}$, and $L_{2\beta}$ are orthogonal LHDs with m factors and $2mk+1$ and $2mk$ runs, respectively. NNOL-Algorithm 2* becomes NNOL-Algorithm 2 if we take $k = 1$.

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

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	−20	−28	24	−18	26	2	−10	47	−13	5	−29	21
2	12	−4	28	−20	25	−26	−18	10	2	48	−21	29	5	−13
3	20	−28	−4	12	26	−6	−14	−22	−30	49	−29	−21	13	5
4	28	20	−12	−4	27	14	−6	30	−22	50	−7	−15	−23	−31
5	4	12	20	28	28	22	−30	−6	14	51	15	−7	31	−23
6	−12	4	−28	20	29	30	22	−14	−6	52	23	−31	−7	15
7	−20	28	4	−12	30	6	14	22	30	53	31	23	−15	−7
8	−28	−20	12	4	31	−14	6	−30	22	54	7	15	23	31
9	−8	−16	−24	−32	32	−22	30	6	−14	55	−15	7	−31	23
10	16	−8	32	−24	33	−30	−22	14	6	56	−23	31	7	−15
11	24	−32	−8	16	34	−3	−11	−19	−27	57	−31	−23	15	7
12	32	24	−16	−8	35	11	−3	27	−19	58	−9	−17	−25	−33
13	0	0	0	0	36	19	−27	−3	11	59	17	−9	33	−25
14	8	16	24	32	37	27	19	−11	3	60	25	−33	−9	17
15	−16	8	−32	24	38	3	11	19	27	61	33	25	−17	−9
16	−24	32	8	−16	39	−11	3	−27	19	62	9	17	25	33
17	−32	−24	16	8	40	−19	27	3	−11	63	−17	9	−33	25
18	−2	−10	−18	−26	41	−27	−19	11	3	64	−25	33	9	−17
19	10	−2	26	−18	42	−5	−13	−21	−29	65	−33	−25	17	9
20	18	−26	−2	10	43	13	−5	29	−21	66	1	1	1	1
21	26	18	−10	−2	44	21	−29	−5	13	67	−1	−1	−1	−1
22	2	10	18	26	45	29	21	−13	−5					
23	−10	2	−26	18	46	5	13	21	29					

Note: The H_α, H_β, H_2, H_3 and H correspond to runs 1−8, 9−17, 1−17, 1−33 and 1−67, respectively.

Example 5 ($m = 4$)**.** For $a = 3$, consider the vectors $A_i^b = b + ai$ for $i = 1, 2, 3, 4$ in Corollary 1 with zero PAF. We can construct nested nearly orthogonal $L((24k+3, 8k+1), 4)$ for any positive integer k. Without loss of generality, we take $k = 1$, so $b = 1, 0, -1$. With the orthogonal matrices

$$D_1 = \begin{pmatrix} 4 & 7 & 10 & 13 \\ -7 & 4 & -13 & 10 \\ -10 & 13 & 4 & -7 \\ -13 & -10 & 7 & 4 \end{pmatrix}, \quad D_0 = \begin{pmatrix} 3 & 6 & 9 & 12 \\ -6 & 3 & -12 & 9 \\ -9 & 12 & 3 & -6 \\ -12 & -9 & 6 & 3 \end{pmatrix},$$

$$D_{-1} = \begin{pmatrix} 2 & 5 & 8 & 11 \\ -5 & 2 & -11 & 8 \\ -8 & 11 & 2 & -5 \\ -11 & -8 & 5 & 2 \end{pmatrix},$$

a nested nearly orthogonal $L((27, 9), 4)$ can be obtained as $(L_1; L_{2\alpha})$, according to NNOL-Algorithm 2, where $L_1 = (-D_0^T, 0_4, D_0^T, -D_{-1}^T, D_{-1}^T, -D_1^T, D_1^T, -1_4, 1_4)^T$ is a nearly orthogonal $L(27, 4)$ with correlation $\rho_{uv} = 1/819$, and $L_{2\alpha} = (-D_0^T, 0_4, D_0^T)^T$ is an orthogonal $L(9, 4)$.

Table 3. The nested nearly orthogonal LHDs with 4 factors and $24k+3$ runs in Example 5.

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	−15	−18	−21	−24	18	−2	−5	−8	−11	34	−16	−19	−22	−25
2	18	−15	24	−21	19	5	−2	11	−8	35	19	−16	25	−2
3	21	−24	−15	18	20	8	−11	−2	5	36	22	−25	−16	19
4	24	21	−18	−15	21	11	8	−5	−2	37	25	22	−19	−16
5	−3	−6	−9	−12	22	2	5	8	11	38	16	19	22	25
6	6	−3	12	−9	23	−5	2	−11	8	39	−19	16	−25	22
7	9	−12	−3	6	24	−8	11	2	−5	40	−22	25	16	−19
8	12	9	−6	−3	25	−11	−8	5	2	41	−25	−22	19	16
9	0	0	0	0	26	−4	−7	−10	−13	42	−14	−17	−20	−23
10	3	6	9	12	27	7	−4	13	−10	43	17	−14	23	−20
11	−6	3	−12	9	28	10	−13	−4	7	44	20	−23	−14	17
12	−9	12	3	−6	29	13	10	−7	−4	45	23	20	−17	−14
13	−12	−9	6	3	30	4	7	10	13	46	14	17	20	23
14	15	18	21	24	31	−7	4	−13	10	47	−17	14	−23	20
15	−18	15	−24	21	32	−10	13	4	−7	48	−20	23	14	−17
16	−21	24	15	−18	33	−13	−10	7	4	49	−23	−20	17	14
17	−24	−21	18	15						50	−1	−1	−1	−1
										51	1	1	1	1

Note: L_1 corresponds to runs 5–13, 18–33 and 50–51; $L_{2\alpha}$ corresponds to runs 5–13; L'_1 corresponds to runs 1–51; $L'_{2\alpha}$ corresponds to runs 1–17.

For $k = 2$, $b = 1, 0, -1, 13, 12, 11$. Using D_1, D_0, D_{-1}, and the orthogonal matrices

$$D_{13} = \begin{pmatrix} 16 & 19 & 22 & 25 \\ -19 & 16 & -25 & 22 \\ -22 & 25 & 16 & -19 \\ -25 & -22 & 19 & 16 \end{pmatrix}, \quad D_{12} = \begin{pmatrix} 15 & 18 & 21 & 24 \\ -18 & 15 & -24 & 21 \\ -21 & 24 & 15 & -18 \\ -24 & -21 & 18 & 15 \end{pmatrix},$$

$$D_{11} = \begin{pmatrix} 14 & 17 & 20 & 23 \\ -17 & 14 & -23 & 20 \\ -20 & 23 & 14 & -17 \\ -23 & -20 & 17 & 14 \end{pmatrix},$$

a nested nearly orthogonal $L((51, 17), 4)$ can be obtained as $(L'_1; L'_{2\alpha})$, where $L'_1 = (-D_{12}^T,\ -D_0^T, 0_4, D_0^T, D_{12}^T, -D_{-1}^T, D_{-1}^T, -D_1^T, D_1^T, -D_{13}^T, D_{13}^T, -D_{11}^T, D_{11}^T, -1_4, 1_4)^T$ is a nearly orthogonal $L(51, 4)$ with correlation $\rho_{uv} = 1/5,525$ and $L'_{2\alpha} = (-D_{12}^T, -D_0^T, 0_4, D_0^T, D_{12}^T)^T$ is an orthogonal $L(17, 4)$. The generated nested LHDs are given in Table 3.

Some vectors for constructing such designs are listed in Appendix B. They are obtained by the algorithm provided by Georgiou and Efthimiou (2014). Since any full fold-over design is 3-orthogonal (Georgiou, Koukouvinos, and Liu (2014)),

Table 4. The proposed nested orthogonal and nearly orthogonal LHDs as well as those given in Yang, Liu, and Lin (2014).

	u	$(n_1,\ldots,n_u)$	a	Method
YLL(2014) $m=2^s$, $s\geq 1$	2	$(2am+1,2m+1)$	$a\geq 2$	Theorem 1
	2	$(2am+1,2m)$	$a\geq 2$, even	Theorem 1
	2	$(4m+1,2m)$	$a\geq 2$	Corollary 1
	2	$(4m+1,2m+1)$	$a\geq 2$	Corollary 1
	$s+1$	$(m2^{s+1}+1,m2^s+1,\ldots,4m+1,2m)$	2^s	Theorem 3
	$s+1$	$(m2^{s+1}+1,m2^s+1,\ldots,4m+1,2m+1)$	2^s	Theorem 3
NEW $m=2,4,$ $8,12,16,$ $20,24$	2	$(4am+1,2m+1)$	$a\geq 1$	Theorem 1(i)
	2	$(4am+1,2m)$	$a\geq 1$	Theorem 1(i)
	2	$(2am+1,2m)$	$a\geq 2$, even	Theorem 1(ii)
	2	$(2am+1,2m+1)$	$a\geq 2$	Theorem 1(ii)
	2	$(4m+1,2m+1)$	$a\geq 2$	Theorem 1(ii)
	2	$(4m+1,2m)$	$a\geq 2$, even	Theorem 1(ii)
	2	$(4m+1,2m)$	$a\geq 1$	Theorem 1(i)
	2	$(4m+1,2m+1)$	$a\geq 1$	Theorem 1(i)
	2	$(4am+3,2m+1)^*$	$a\geq 2$	Theorem 2(i)
	2	$(4am+3,2m)^*$	$a\geq 2$	Theorem 2(i)
	2	$(2am+3,2m)^*$	$a\geq 2$, even	Theorem 2(ii)
	2	$(2am+3,2m+1)^*$	$a\geq 2$	Theorem 2(ii)
	$t+3$	$(4am+1,2^{t+2}m+1,2^{t+1}m+1,\ldots,4m+1,2m)$	$a\neq 2^q$, even	Section 5
	$t+3$	$(4am+1,2^{t+2}m+1,2^{t+1}m+1,\ldots,4m+1,2m+1)$	$a\neq 2^q$, even	Section 5
	$t+3$	$(4am+3,2^{t+2}m+1,2^{t+1}m+1,\ldots,4m+1,2m)^*$	$a\neq 2^q$, even	Section 5
	$t+3$	$(4am+3,2^{t+2}m+1,2^{t+1}m+1,\ldots,4m+1,2m+1)^*$	$a\neq 2^q$, even	Section 5
	$t+2$	$(4am+1,2^{t+1}m+1,2^tm+1,\ldots,4m+1,2m)$	$a=2^q$	Section 5
	$t+2$	$(4am+1,2^{t+1}m+1,2^tm+1,\ldots,4m+1,2m+1)$	$a=2^q$	Section 5
	$t+2$	$(4am+3,2^{t+1}m+1,2^tm+1,\ldots,4m+1,2m)^*$	$a=2^q$	Section 5
	$t+2$	$(4am+3,2^{t+1}m+1,2^tm+1,\ldots,4m+1,2m+1)^*$	$a=2^q$	Section 5

Note: The symbol * in the third column means that the corresponding design is a nested nearly orthogonal LHD; $t=\max\{i:2^i|a\}$, $x|y$ denotes y is divisible by x; $q\geq 2$; Yang, Liu, and Lin (2014) refers to Yang, Liu, and Lin (2014).

the resulting nested orthogonal and nearly orthogonal LHDs satisfy the desirable property that the sum of the elementwise product of any three columns is zero. Such designs guarantee that the estimate of each linear effect is uncorrelated with all second-order effects, in addition to exactly or nearly uncorrelated with all other linear effects.

The new nested orthogonal LHDs (nested nearly orthogonal LHDs), as well as the nested orthogonal LHDs given by Yang, Liu, and Lin (2014), are listed in Table 4. It can be seen there that the designs we constructed have a flexible number of runs and factors. In particular, we can construct nested orthogonal LHDs with 12, 20, and 24 factors and nested nearly orthogonal LHDs with 2, 4, 8, 12, 16, 20, and 24 factors and a low correlation between any two distinct columns.

Acknowledgements

The authors thank Editor Professor Ruey S. Tsay, an associate editor, and two referees for their valuable comments and suggestions that have resulted in improvements in the paper. This work was supported by the National Natural Science Foundation of China (Grant Nos. 11271205, 11271355, 11431006, 11471172, and 11401321), the Specialized Research Fund for the Doctoral Program of Higher Education of China (Grant No. 20130031110002), the "131" Talents Program of Tianjin, and National Security Agent via Grant No. H98230-15-1-0253.

Appendix A: Proofs

A.1. Proof of Theorem 1

Without loss of generality, we only consider $r = 4$ (four vectors $A_1^b, A_2^b, A_3^b, A_4^b$). For $r = 2$ or 8, the proof is similar.

(i) It is obvious that $L_{2\alpha} \subset L_1$ and $L_{2\beta} \subset L_1$ hold from the definitions of L_1, $L_{2\alpha}$, and $L_{2\beta}$ in NOL-Algorithm 1. We show that the entries of each column of L_1, $L_{2\alpha}$, and $L_{2\beta}$ are equally spaced. It is easy to verify that the absolute values of the entries in each column of E are $\{1, 2, \ldots, 2am\}$. This indicates that the entries in each column of L_1 are $\{0, \pm 1, \pm 2, \ldots, \pm 2am\}$. From the definition of D_b, the entries in each column of $L_{2\alpha}$ and $L_{2\beta}$ are $\{\pm a, \pm 3a, \ldots, \pm(2m-1)a\}$ and $\{0, \pm 2a, \pm 4a, \ldots, \pm 2am\}$, respectively. Thus, both $(L_1; L_{2\alpha})$ and $(L_1; L_{2\beta})$ are nested LHDs. The orthogonality of $L_1, L_{2\alpha}$, and $L_{2\beta}$ can be easily obtained by noting that the set of vectors $\{A_1^b, A_2^b, A_3^b, A_4^b\}$ has zero PAF.

(ii) The proof of (ii) is similar to that of (i) and is thus omitted.

A.2. Proof of Theorem 2

Similar to the proof of Theorem 1, we only consider $r = 4$.

(i) It is obvious that $L_{2\alpha} \subset L_1$ and $L_{2\beta} \subset L_1$ hold from the definitions of L_1, $L_{2\alpha}$, and $L_{2\beta}$ in NNOL-Algorithm 1.

We show that the entries of each column of L_1, $L_{2\alpha}$, and $L_{2\beta}$ are equally spaced. From the definition of D_b and E, it is easy to verify that the entries in each column of L_1, $L_{2\alpha}$ and $L_{2\beta}$ are $\{0, \pm 1, \pm 2, \ldots, \pm(2am+1)\}$, $\{\pm a, \pm 3a, \ldots, \pm(2m-1)a\}$, and $\{0, \pm 2a, \pm 4a, \ldots, \pm 2am\}$, respectively. Thus, both $(L_1; L_{2\alpha})$ and $(L_1; L_{2\beta})$ are nested LHDs.

From the orthogonality of D_b, we have

$$
\begin{aligned}
L_1^T L_1 &= 2E^T E + 2J_m = 2\Big(\sum_{i=1}^{2am+1} i^2 - 1\Big) I_m + 2J_m \\
&= \Big(\frac{(2am+1)(2am+2)(4am+3)}{3} - 2\Big) I_m + 2J_m,
\end{aligned}
$$

where I_m is the identity matrix of order m and J_m is the $m \times m$ matrix with all entries unity. Obviously $\rho_{uv} = 6/[(2am+1)(2am+2)(4am+3)]$ for any two distinct columns u and v of L_1. Thus, L_1 is a nearly orthogonal LHD. From the definition of D_b, we know that

$$L_{2\alpha}^T L_{2\alpha} = \frac{2a^2m(2m+1)(2m-1)}{3} I_m \text{ and } L_{2\beta}^T L_{2\beta} = \frac{2a^2m(2m+1)(2m+2)}{3} I_m.$$

Thus we obtain the near orthogonality of L_1 and the orthogonality of $L_{2\alpha}$ and $L_{2\beta}$.

(ii) Similar to the proof of (i), consider L_1, $L_{2\alpha}$, and $L_{2\beta}$ given in NNOL-Algorithm 2. Since the entries of L_1 are $\{0, \pm 1, \ldots, \pm(am+1)\}$, $\rho_{uv} = 6/[(am+1)(am+2)(2am+3)]$, where u and v are any two distinct columns of L_1. Following the proof of (i), $(L_1; L_{2\alpha})$ is the desired nested nearly orthogonal $L((2am+3, 2m+1), m)$ and $(L_1; L_{2\beta})$ is a nested nearly orthogonal $L((2am+3, 2m), m)$ with correlation $\rho_{uv} = 6/[(am+1)(am+2)(2am+3)]$, for any two distinct columns u and v of L_1.

Appendix B: Vectors with Zero PAF Used in the Algorithms

Table B.1. General vectors with zero PAF used in NOL-Algorithm 1 and NNOL-Algorithm 1.

Number of factors	Needed vectors
2	$A_1^b = (b+a)$, $A_2^b = (b+3a)$
4	$A_1^b = (b+a)$, $A_2^b = (b+3a)$, $A_3^b = (b+5a)$, $A_4^b = (b+7a)$
8	$A_i^b = (b+(2i-1)a)$, $i = 1, \ldots, 8$
12	$A_1^b = (b+15a, -(b+5a), b+19a)$, $A_2^b = (b+17a, -(b+21a), b+23a)$, $A_3^b = (b+a, b+3a, -(b+7a))$, $A_4^b = (b+9a, b+11a, b+13a)$
16	$A_1^b = (b+a, b+3a)$, $A_2^b = (b+5a, -(b+7a))$, $A_3^b = (b+9a, -(b+11a))$, $A_4^b = (b+13a, b+15a)$, $A_5^b = (b+17a, -(b+19a))$, $A_6^b = (b+21a, b+23a)$, $A_7^b = (b+25a, b+27a)$, $A_8^b = (b+29a, -(b+31a))$
20	$A_1^b = (b+21a, b+5a, -(b+27a), b+29a, b+23a)$, $A_2^b = (b+25a, b+31a, b+33a, b+35a, -(b+37a))$, $A_3^b = (b+39a, b+a, -(b+3a), -(b+7a), -(b+9a))$, $A_4^b = (b+11a, b+13a, -(b+15a), b+17a, -(b+19a))$
24	$A_1^b = (b+a, b+27a, b+3a)$, $A_2^b = (b+5a, b+7a, -(b+9a))$, $A_3^b = (b+11a, -(b+13a), -(b+15a))$, $A_4^b = (b+17a, b+19a, -(b+21a))$, $A_5^b = (b+23a, -(b+25a), b+29a)$, $A_6^b = (b+31a, b+33a, -(b+35a))$, $A_7^b = (b+37a, b+39a, b+41a)$, $A_8^b = (b+43a, b+45a, -(b+47a))$

Table B.2. General vectors with zero PAF used in NOL-Algorithm 2 and NNOL-Algorithm 2.

Number of factors	Needed vectors
2	$A_1^b=(b+a),\ A_2^b=(b+2a)$
4	$A_1^b=(b+a),\ A_2^b=(b+2a),\ A_3^b=(b+3a),\ A_4^b=(b+4a)$
8	$A_i^b=(b+ia),\ i=1,\dots,8$
12	$A_1^b=(b+8a,-(b+3a),b+10a),\ A_2^b=(b+9a,-(b+11a),b+12a),$ $A_3^b=(b+a,b+2a,-(b+4a)),\ A_4^b=(b+5a,b+6a,b+7a)$
16	$A_1^b=(b+a,b+2a),\ A_2^b=(b+3a,-(b+4a)),\ A_3^b=(b+5a,-(b+6a)),$ $A_4^b=(b+7a,b+8a),\ A_5^b=(b+9a,-(b+10a)),\ A_6^b=(b+11a,b+12a),$ $A_7^b=(b+13a,b+14a),\ A_8^b=(b+15a,-(b+16a))$
20	$A_1^b=(b+11a,b+3a,-(b+14a),b+15a,b+12a), A_2^b=(b+13a,$ $b+16a,b+17a,b+18a,-(b+19a)),\ A_3^b=(b+20a,b+a,-(b+2a),$ $-(b+4a),-(b+5a)),\ A_4^b=(b+6a,b+7a,-(b+8a),b+9a,-(b+10a))$
24	$A_1^b=(b+a,b+14a,b+2a),\ A_2^b=(b+3a,b+4a,-(b+5a)),$ $A_3^b=(b+6a,-(b+7a),-(b+8a)),\ A_4^b=(b+9a,b+10a,-(b+11a)),$ $A_5^b=(b+12a,-(b+13a),b+15a),\ A_6^b=(b+16a,b+17a,-(b+18a)),$ $A_7^b=(b+19a,b+20a,b+21a),\ A_8^b=(b+22a,b+23a,-(b+24a))$

Appendix C: Constructed Designs in Example 2

C.1. D_0 and D_{-1} in Example 2

D_0

22	6	−28	30	24	−38	36	34	32	26	−10	−8	−4	2	40	−20	18	−16	14	12
24	22	6	−28	30	36	34	32	26	−38	−8	−4	2	40	−10	18	−16	14	12	−20
30	24	22	6	−28	34	32	26	−38	36	−4	2	40	−10	−8	−16	14	12	−20	18
−28	30	24	22	6	32	26	−38	36	34	2	40	−10	−8	−4	14	12	−20	18	−16
6	−28	30	24	22	26	−38	36	34	32	40	−10	−8	−4	2	12	−20	18	−16	14
38	−36	−34	−32	−26	22	6	−28	30	24	−14	16	−18	20	12	2	−4	−8	−10	40
−36	−34	−32	−26	38	24	22	6	−28	30	16	−18	20	12	−14	−4	−8	−10	40	2
−34	−32	−26	38	−36	30	24	22	6	−28	−18	20	12	−14	16	−8	−10	40	2	−4
−32	−26	38	−36	−34	−28	30	24	22	6	20	12	−14	16	−18	−10	40	2	−4	−8
−26	38	−36	−34	−32	6	−28	30	24	22	12	−14	16	−18	−29	40	2	−4	−8	−10
10	8	4	−2	−40	14	−16	18	−20	12	22	6	−28	30	24	−32	−34	−36	38	−26
8	4	−2	−40	10	−16	18	−20	12	14	24	22	6	−28	30	−34	−36	38	−26	−32
4	−2	−40	10	8	18	−20	12	14	−16	30	24	22	6	−28	−36	38	−26	−32	−34
−2	−40	10	8	4	−20	12	14	−16	18	−28	30	24	22	6	38	−26	−32	−34	−36
−40	10	8	4	−2	12	14	−16	18	−20	6	−28	30	24	22	−26	−32	−34	−36	38
20	−18	16	−14	−12	−2	4	8	10	−40	32	34	36	−38	26	22	6	−28	30	24
−18	16	−14	−12	20	4	8	10	−40	−2	34	36	−38	26	32	24	22	6	−28	30
16	−14	−12	20	−18	8	10	−40	−2	4	36	−38	26	32	34	30	24	22	6	−28
−14	−12	20	−18	16	10	−40	−2	4	8	−38	26	32	34	36	−28	30	24	22	6
−12	20	−18	16	−14	−40	−2	4	8	10	26	32	34	36	−38	6	−28	30	24	22

D_{-1}

21	5	−27	29	23	−37	35	33	31	25	−9	−7	−3	1	39	−19	17	−15	13	11
23	21	5	−27	29	35	33	31	25	−37	−7	−3	1	39	−9	17	−15	13	11	−19
29	23	21	5	−27	33	31	25	−37	35	−3	1	39	−9	−7	−15	13	11	−19	17
−27	29	23	21	5	31	25	−37	35	33	1	39	−9	−7	−3	13	11	−19	17	−15
5	−27	29	23	21	25	−37	35	33	31	39	−9	−7	−3	1	11	−19	17	−15	13
37	−35	−33	−31	−25	21	5	−27	29	23	−13	15	−17	19	11	1	−3	−7	−9	39
−35	−33	−31	−25	37	23	21	5	−27	29	15	−17	19	11	−13	−3	−7	−9	39	1
−33	−31	−25	37	−35	29	23	21	5	−27	−17	19	11	−13	15	−7	−9	39	1	−3
−31	−25	37	−35	−33	−27	29	23	21	5	19	11	−13	15	−17	−9	39	1	−3	−7
−25	37	−35	−33	−31	5	−27	29	23	21	11	−13	15	−17	19	39	1	−3	−7	−9
9	7	3	−1	−39	13	−15	17	−19	11	21	5	−27	29	23	−31	−33	−35	37	−25
7	3	−1	−39	9	−15	17	−19	11	13	23	21	5	−27	29	−33	−35	37	−25	−31
3	−1	−39	9	7	17	−19	11	13	−15	29	23	21	5	−27	−35	37	−25	−31	−33
−1	−39	9	7	3	−19	11	13	−15	17	−27	29	23	21	5	37	−25	−31	−33	−35
−39	9	7	3	−1	11	13	−15	17	−19	5	−27	29	23	21	−25	−31	−33	−35	37
19	−17	15	−13	−11	−1	3	7	9	−39	31	33	35	−37	25	21	5	−27	29	23
−17	15	−13	−11	19	3	7	9	−39	−1	33	35	−37	25	31	23	21	5	−27	29
15	−13	−11	19	−17	7	9	−39	−1	3	35	−37	25	31	33	29	23	21	5	−27
−13	−11	19	−17	15	9	−39	−1	3	7	−37	25	31	33	35	−27	29	23	21	5
−11	19	−17	15	−13	−39	−1	3	7	9	25	31	33	35	−37	5	−27	29	23	21

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Department of Statistics, Tianjin University of Finance and Economics, Tianjin 300222, China.

E-mail: yangxue_302@163.com

LPMC and Institute of Statistics, Nankai University, Tianjin 300071, China.

E-mail: jfyang@nankai.edu.cn

Department of Statistics, The Pennsylvania State University, University Park, PA 16802, USA.

E-mail: DKL5@psu.edu

LPMC and Institute of Statistics, Nankai University, Tianjin 300071, China.

E-mail: mqliu@nankai.edu.cn

(Received January 2014; accepted November 2015)