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| **Notice:** Accepted version subject to English editing. |
CONSTRUCTION OF ORTHOGONAL SYMMETRIC LATIN HYPERCUBE DESIGNS

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¹Nankai University, ²Northeast Normal University
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Abstract: Latin hypercube designs (LHDs) have found wide application in computer experiments. It is known that orthogonal LHDs guarantee the orthogonality between all linear effects, and symmetric LHDs ensure the orthogonality between linear and second-order effects. In this paper, we propose a construction method for orthogonal symmetric LHDs. Most resulting LHDs can accommodate the maximum number of factors, thus can study many more factors than existing ones. Moreover, several methods for constructing nearly orthogonal symmetric LHDs are also provided. All the constructed orthogonal and nearly orthogonal LHDs could be utilized to generate more nearly orthogonal symmetric LHDs. A detailed comparison with existing designs shows that the resulting designs have more flexible and economical run sizes and have many desirable design properties.

Key words and phrases: Computer experiment, correlation, second-order effect, symmetric Latin hypercube design.

1. Introduction

Computer models and simulators are used as a way to explore complex physical systems. With the computational power increasing, simulations can be quite large and extremely complex. Many simulations contain thousands of input variables, a substantial number of which may be significant (see for example, Cioppa and Lucas (2007), and Gramacy et al. (2015)). Simulations are used not only to screen significant factors, but also to understand and reason about these complex systems and processes. To efficiently explore these simulations, we need experimental designs that allow us to screen a large number of input variables by fitting commonly used linear-main-effects
models with (nearly) uncorrelated coefficient estimates, while providing flexibility to fit complex models on selected dominant factors.

Orthogonal Latin hypercube designs (LHDs) are commonly used for this goal. An orthogonal LHD is an LHD with centered levels and zero inner product between any two distinct columns. Obviously, orthogonal LHDs allow uncorrelated estimates of linear main effects. They also provide some space-filling property for fitting complex models, say, Gaussian process models, on selected factors. Detailed justifications can be found in Owen (1994), Joseph and Hung (2008), Lin and Tang (2015), among others. A number of methods have been proposed to construct orthogonal and nearly orthogonal LHDs, see e.g., Beattie and Lin (1997), Steinberg and Lin (2006), Pang, Liu, and Lin (2009), Georgiou (2009), Lin, Mukerjee, and Tang (2009), Sun, Liu, and Lin (2009, 2010), Lin et al. (2010), Georgiou and Stylianou (2011), Yang and Liu (2012), Ai, He, and Liu (2012), Yin and Liu (2013), Georgiou and Efthimiou (2014), Efthimiou, Georgiou, and Liu (2015), Wang et al. (2015) and the references therein.

Orthogonality may not be sufficient for fitting a linear-main-effects model when second-order effects (i.e., quadratic effects or bilinear interactions) are present because the estimates of linear main effects may be biased by nonnegligible second-order effects. This paper constructs orthogonal symmetric LHDs (OSLHDs), which allow uncorrelated estimates of linear main effects while making sure these estimates are not biased by second-order effects (cf., Ye (1998)). A design is called symmetric, if for any row \(d\), \(-d\) is also one of the rows in the design. Ye, Li, and Sudjianto (2000) showed that symmetry is also an ideal property for fitting Gaussian process models because symmetric designs are more space-filling and perform better under the maximum entropy criterion (Shewry and Wynn (1987)). Some of the orthogonal LHDs constructed by Cioppa and Lucas (2007), Sun, Liu, and Lin (2009, 2010), and Yang and Liu (2012) are symmetric. However, they are only available for very limited sizes: \(c2^{r+1}\) or \(c2^{r+1} + 1\) runs for at most \(2^r\) factors, where \(c\) and \(r\) are positive integers. Georgiou (2009) constructed OSLHDs with 4, 5, 8, 9, 16, 17 runs. The OSLHDs in Georgiou and Stylianou (2011) and Georgiou and Efthimiou (2014) are only able to accommodate 32 or less factors.

In this paper, methods for constructing orthogonal (or nearly orthogonal) symmet-
ric LHDs are proposed. In particular, the resulting OSLHDs may have \(q^d\) runs and \((q^d - 1)/2\) factors, where \(q\) is an odd prime and \(d = 2^c\) with \(c\) being any positive integer. Note that the number of factors, \((q^d - 1)/2\), is indeed the maximum possible value. Hence, the constructed OSLHDs have larger factor-to-run ratios and are more economical than existing OSLHDs. The newly constructed nearly orthogonal symmetric LHDs (NOSLHDs) with \(q^d + i\) runs (where \(i = -1, 0, 1, 2\) and \(d\) is any positive integer) have low correlations between any two distinct columns and also high factor-to-run ratios.

This paper is organized as follows. Section 2 provides the main construction method and theoretical result of the paper. OSLHDs and NOSLHDs are then constructed in Sections 3 and 4, respectively. A detailed comparison between the proposed methods and some existing ones is made in Section 5. It is shown that the proposed methods are able to construct many new OSLHDs and NOSLHDs with more flexible run sizes and larger numbers of factors. Concluding remarks are given in Section 6. For clarity, all proofs are deferred to the Appendix.

2. Main Result

Throughout the paper, \(q\) is an odd prime number. Let \(GF(q) = \{0, \ldots, q - 1\}\) and \(GF(q)[x] = \{a_0 + a_1 x + \cdots + a_{d-1} x^{d-1}, a_0, \ldots, a_d \in GF(q)\}\). A \(q^d\)-run full factorial design has \(d\) columns \(1, \ldots, d\). Each column, or a generated column, of \(1, \ldots, d\), can be denoted by \(1^{a_0} \cdots x^{d-1}d\) for some \(a_0, \ldots, a_d \in GF(q)\) and corresponds to a nonzero element \(a_0 + a_1 x + \cdots + a_{d-1} x^{d-1}\) in \(GF(q)[x]\). Note that each nonzero element in \(GF(q)[x]\) can also be expressed as \(x^k\) modulo a primitive polynomial \(f(x)\) over \(GF(q)[x]\) for \(k \in \{0, \ldots, q^d - 1\}\). Let \(b = [(q^d - 1)/(d(q - 1))]\), where \(\lfloor c \rfloor\) denotes the largest integer less than or equal to \(c\). As shown in Steinberg and Lin (2006) and Pang, Liu, and Lin (2009), the corresponding columns of the first \(m = bd\) nonzero elements of \(GF(q)[x], x^0, x^1, \ldots, x^{m-1}\) modulo \(f(x)\), form a regular design, denoted by \(D\). Any \(d\) consecutive columns of \(D\) are a full factorial design. Based on this property of \(D\), we propose the following new algorithm for constructing symmetric LHDs.

Algorithm 1 (Construction of symmetric LHDs).

Step 1. Given \(q\) and \(d\), obtain a regular design \(D\) with \(n = q^d\) runs and \(m = bd\) factors...
such that any $d$ consecutive columns of $D$ form a full factorial design.

**Step 2.** Derive a symmetric $LHD(q, p)$ $B = (b_{ij})$ with levels $\{-(q-1)/2, -(q-3)/2, \ldots, (q-1)/2\}$ and $b_{ij} = -b_{q+1-i,j}$, where $LHD(q, p)$ denotes an LHD with $q$ runs and $p$ factors.

**Step 3.** For $j = 1, \ldots, p$, obtain an $n \times m$ matrix $D^{(j)}$ from $D$ by replacing the levels $0, \ldots, q-1$ of $D$ with $b_{(q+1)/2,j}, \ldots, b_{q,j}, b_1, \ldots, b_{(q-1)/2,j}$, respectively.

**Step 4.** Let $T_d$ be a matrix of order $d$ comprised of columns of permutations of $\{1, q, \ldots, q^{d-1}\}$ (up to sign changes). For $j = 1, \ldots, p$, let $L^{(j)} = D^{(j)}T$ where $T = \text{diag}\{T_d, \ldots, T_d\}$ with $T_d$ repeating $b$ times.

**Step 5.** The resulting design matrix is then

$$L = (L^{(1)}, \ldots, L^{(p)}).$$

(2.1)

For any matrix $X = (x_1, \ldots, x_m)$ where $x_i$ is the $i$th column of $X$ for $i = 1, \ldots, m$, define $\rho_{ij}(X) = x_i^T x_j / (x_i^T x_i x_j^T x_j)^{1/2}$ as the correlation between the $i$th and $j$th columns, and $C_X = (\rho_{ij}(X))$ as the correlation matrix of $X$.

**Theorem 1.** (i) The matrix $L$ in (2.1) is a symmetric $LHD(n, mp)$ with levels $\{-(n-1)/2, -(n-3)/2, \ldots, (n-1)/2\}$.

(ii) The correlation matrix of $L$ in (2.1) is given by $C_L = C_B \otimes I_b \otimes C_{T_d}$, where $I_b$ is the identity matrix of order $b$ and $\otimes$ denotes the Kronecker product.

Theorem 1 not only declares that the design constructed by the proposed algorithm is a symmetric LHD, but also gives an insight into its correlation structure. By Theorem 1 an OSLHD can be obtained by carefully choosing the design $B$ and the matrix $T_d$.

**Example 1.** Let $q = 5$, $d = 2$, and $D$ be the $5^{6-4}$ regular factorial design shown in Table 1. Any two columns of $D$ form a $5^2$ full factorial design. Suppose $B$ is the OSLHD$(5,2)$ constructed by Ye (1998):

$$B = \begin{pmatrix}
-2 & -1 & 0 & 1 & 2 \\
-1 & 2 & 0 & -2 & 1
\end{pmatrix}^T.$$
ORTHOGONAL SYMMETRIC LATIN HYPERCUBE DESIGNS

Table 1: The regular design $D$ (in transpose) in Example 1

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and

$$T_2 = \begin{pmatrix} 5 & -1 \\ 1 & 5 \end{pmatrix}.$$  

Then $D^{(1)}$ and $D^{(2)}$ can be obtained by replacing the levels 0, . . . , 4 of $D$ with the entries in the first and second column of $B$ respectively, following the replacing rule specified in Step 3 of Algorithm 1. Let $L^{(k)} = D^{(k)}T$ with $T = \text{diag}(T_2, T_2, T_2)$, for $k = 1, 2$. Then it can be easily checked that $L = (L^{(1)}, L^{(2)})$, which is shown in Table 2 is an OSLHD(25, 12).

Table 2: The design $L = (L^{(1)}, L^{(2)})$ (in transpose) in Example 1

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<th>-12 -7 -2 3 8 -11 -6 -1 4 9 -10 -50 5 10 -9 -4 1 6 11 -8 -3 2 7 12</th>
<th>-12 -7 -2 3 8 -11 -6 -1 4 9 -10 -50 5 10 -9 -4 1 6 11 -8 -3 2 7 12</th>
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<tr>
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<td>3 -5 12 -1 -9 2 -11 6 -7 -10 -4 80 -8 4 -10 7 -6 11 -2 9 1 -12 5 -3</td>
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<td>-11 1 8 -5 7 10 -3 4 -9 -2 6 -120 12 -6 2 9 -4 3 -10 -7 5 -8 -1 11</td>
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Example 1 is a typical illustration for constructing an OSLHD from the proposed algorithm. By choosing different $B$’s and $T_i$’s, more OSLHDs can be constructed, which will be discussed in the next section.
Remark 1. Note that for the case of $d = 2$ and

$$T_2 = \begin{pmatrix} 1 & -q \\ q & 1 \end{pmatrix},$$

the proposed construction method is a special case of the method of Lin, Mukerjee, and Tang (2009). However, their designs may not be symmetric. The difference is that we use a symmetric LHD (the design $B$) in Step 2, and organize its row-order in Step 3, such that the resulting design $L$ can be symmetric with better properties.

3. Construction of OSLHDs

For the construction of OSLHDs, the following result is directly from Theorem 1.

Corollary 1. If $B$ is orthogonal and $T_d$ is column-orthogonal, i.e., $T_d^T T_d = a_d I_d$ with $a_d = (q^{2d} - 1)/(q^2 - 1)$, then $L$ in (2.1) is orthogonal.

From Corollary 1 an OSLHD($q,p$) $B$ and a column-orthogonal $T_d$ are needed for constructing an OSLHD($q^d, bdp$), where $b = \lfloor(q^d - 1)/(d(q - 1))\rfloor$. For $d = 2^c$ with $c = 1, 2, \ldots$, the $T_d$ can be obtained recursively (Pang, Liu, and Lin (2009)) by letting $T_{2^0} = 1$ and

$$T_{2^c} = \begin{pmatrix} q^{2^{c-1}} T_{2^{c-1}} & -T_{2^{c-1}} \\ T_{2^{c-1}} & q^{2^{c-1}} T_{2^{c-1}} \end{pmatrix}. \quad (3.1)$$

Note that $(q^d - 1)/(d(q - 1))$ is an integer and $b = (q^d - 1)/(d(q - 1))$ for $d = 2^c$. For $q = 3$, the choice of $B$ can only be $(-1, 0, 1)^T$. In this case, the construction described in the last section yields OSLHD($n,m$’s with $n = 3^d$ and $m = (n - 1)/2$, for example OSLHD(9, 4) and OSLHD(81, 40). Note that an OSLHD($n,m$) is second-order orthogonal which satisfies that $m \leq \lfloor n/2 \rfloor$ (see Theorem 3 of Sun, Liu, and Lin (2009)). OSLHD($n,m$’s with $m = \lfloor n/2 \rfloor$ are called saturated. The following results can be straightforwardly obtained.

Proposition 1. For $q = 3$, $d = 2^c$, and $T_d$ defined in (3.1), the OSLHD $L$ constructed in (2.1) is saturated.

For $q \geq 5$, if $B$ is saturated (i.e., $B$ has $p = (q - 1)/2$ factors), then $L$ has $(q^d - 1)/2$ columns and is also saturated.
Proposition 2. If \( B \) is saturated and \( T_d \) is defined in (3.1), the OSLHD \( L \) constructed in (2.1) is saturated.

Obviously, the OSLHD(25,12) obtained in Example \([\text{I}]\) is saturated. In addition, with \( T_2 \) and \( T_4 \) in (3.1), and the OSLHD(5,2) and OSLHD(17,8) constructed by Yang and Liu (2012), the proposed construction yields saturated OSLHD(25,12), OSLHD(625,312) and OSLHD(289,144). As another example, we could have the OSLHD(11,3) and OSLHD(13,3) shown in Table 3 which are obtained by computer search and are apparently new. With \( T_2 \) defined in (3.1), we can obtain OSLHD(121,36) and OSLHD(169,42). Though they are not saturated, they are new and can also accommodate many factors.

Table 3: Newly searched OSLHD(11,3) and OSLHD(13,3) (in transpose).

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4. Construction of NOSLHDs

For given \( q \) and \( p \), if there does not exist any OSLHD(\( q,p \)) as the design \( B \) in the proposed method, and/or there does not exist a column-orthogonal matrix \( T_d \), a nearly orthogonal LHD for \( B \) and a nearly column-orthogonal matrix for \( T_d \) (cf., Sun, Pang, and Liu (2011)) can be used instead. For an \( n \times m \) matrix \( X \), the near orthogonality is usually assessed by \( \rho_M(X) = \max_{i<j} |\rho_{ij}(X)| \) and \( \rho_{\text{ave}}^2(X) = \sum_{i<j} \rho_{ij}^2(X)/(m(m-1)/2) \). The \( \rho_M \) measures the maximum correlation, and the \( \rho_{\text{ave}}^2 \) measures both magnitudes and sparsity of the correlations. The following result from Theorem \([\text{I}]\) gives the values for \( \rho_M \) and \( \rho_{\text{ave}}^2 \) of the resulting design \( L \) in (2.1).
Corollary 2. For $L$ in (2.1), we have

$$
\rho_M(L) = \max \{ \rho_M(B), \rho_M(T_d) \}, \quad \text{and} \quad \rho_{ave}^2(L) = \frac{(d - 1)\rho_{ave}^2(T_d) + (d - 1)(p - 1)\rho_{ave}^2(T_d)\rho_{ave}^2(B) + (p - 1)\rho_{ave}^2(B)}{bdp - 1}.
$$

Butler (2001) constructed optimal LHD($n, m$) for Fourier-polynomial models where $n$ is a prime and $m = (n - 1)/2$. When scaling the levels to $\{- (n - 1)/2, -(n - 3)/2, \ldots, (n - 1)/2\}$, his resulting LHDs are symmetric with low and sparse correlations. With his LHD(11, 5), LHD(13, 6), LHD(19, 9) and LHD(23, 11), and $T_2$ in (3.1), we are able to construct an NOSLHD(121, 60), NOSLHD(169, 84), NOSLHD(361, 180) and NOSLHD(529, 264) with $\rho_M = 0.0909, 0.0989, 0.1053$ and $0.1067$, and $\rho_{ave}^2 = 0.0003, 0.0002, 0.0001$ and 0.0001, respectively.

In addition, through computer search, we find that the matrix

$$
\begin{pmatrix}
1 & 1 & q^2 \\
q & -q^2 & 1 \\
q^2 & q & -q
\end{pmatrix}
$$

is an optimal choice for $T_3$ because it has the minimum $\rho_M$ and $\rho_{ave}^2$ among all choices for $T_3$. By this $T_3$, we can obtain an NOSLHD(27, 12) as follows.

Example 2. Using the primitive polynomial $f(x) = x^3 + 2x + 1$ over $GF(3)[x]$, $x^0, \ldots, x^{11}$ modulo $f(x)$, are $1, x, x^2, 2 + x, 2x + x^2, 2 + x + 2x^2, 1 + x + x^2, 2 + 2x + x^2, 2 + 2x^2, 1 + x, x + x^2, 2 + x + x^2$, respectively, which correspond in order to the twelve columns of the regular factorial design $D$ shown in Table 4. Any 3 consecutive columns of $D$ form a full factorial design. Let $B = (-1, 0, 1)^T$,

$$
T_3 = \begin{pmatrix}
1 & 1 & 9 \\
3 & -9 & 1 \\
9 & 3 & -3
\end{pmatrix}
$$

with correlation matrix

$$
C_T = \begin{pmatrix}
1 & 0.0110 & -0.1648 \\
0.0110 & 1 & -0.0989 \\
-0.1648 & -0.0989 & 1
\end{pmatrix},
$$
Table 4: The regular design $D$ (in transpose) in Example 2.

| 1 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 | 1 2 | 0 1 | 2 0 |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 2 0 | 0 0 | 1 1 | 1 2 | 2 2 | 0 0 | 0 1 | 1 2 | 2 2 | 0 0 | 0 1 | 1 2 | 2 2 | 0 0 | 0 1 | 1 2 | 2 2 | 0 0 | 0 1 | 1 2 | 2 2 | 0 0 |
| 3 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 |
| 1^2 2 | 0 2 | 1 1 | 0 2 | 2 1 | 0 0 | 2 1 | 1 0 | 2 2 | 1 0 | 0 0 | 2 1 | 1 0 | 2 2 | 1 0 | 0 0 | 2 1 | 1 0 | 2 2 | 1 0 | 0 0 |
| 2^2 3 | 0 0 | 0 0 | 2 2 | 2 1 | 1 1 | 1 1 | 1 1 | 0 0 | 0 0 | 2 2 | 2 2 | 2 2 | 1 1 | 1 1 | 0 0 | 0 0 | 2 2 | 2 2 | 2 2 | 1 1 |
| 1^2 23 | 0 2 | 1 1 | 0 2 | 2 1 | 0 2 | 1 0 | 0 2 | 1 0 | 2 1 | 0 2 | 1 0 | 0 2 | 1 0 | 2 1 | 0 2 | 1 0 | 0 2 | 1 0 | 0 2 | 1 0 |
| 123 | 0 1 | 2 1 | 2 0 | 2 0 | 1 1 | 1 1 | 1 1 | 1 1 | 0 1 | 2 2 | 1 1 | 1 1 | 1 1 | 0 1 | 2 2 | 1 1 | 1 1 | 1 1 | 0 1 | 2 2 |
| 12^2 3 | 0 2 | 1 2 | 1 0 | 1 0 | 2 1 | 0 2 | 1 2 | 1 0 | 1 0 | 2 1 | 0 2 | 1 2 | 1 0 | 1 0 | 2 1 | 0 2 | 1 2 | 1 0 | 1 0 |
| 1^2 3^2 | 0 2 | 1 0 | 2 1 | 0 2 | 1 2 | 0 2 | 1 0 | 1 0 | 2 1 | 0 2 | 1 0 | 1 0 | 2 1 | 0 2 | 1 0 | 1 0 | 2 1 |
| 12 | 0 1 | 2 1 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 | 0 2 |
| 23 | 0 0 | 0 0 | 1 1 | 1 2 | 1 1 | 1 1 | 1 2 | 1 2 | 1 1 | 1 1 | 1 2 | 1 2 | 1 1 | 1 1 | 1 2 | 1 2 | 1 1 | 1 1 |
| 1^2 23 | 0 2 | 1 1 | 0 2 | 2 1 | 1 0 | 1 0 | 2 2 | 1 0 | 0 0 | 2 1 | 2 1 | 0 0 | 0 1 | 1 1 |

and $T = \text{diag}\{T_3, T_3, T_3, T_3\}$. Then by Corollary 2 (2.1) leads to an NOSLHD(27, 12), say $L$, with $\rho_M(L) = \rho_M(T_3) = 0.1648$ and $\rho_{\text{ave}}^2(L) = 0.0022$. By Theorem 1 the correlation matrix of $L$ is given by $C_L = \text{diag}\{C_T, C_T, C_T, C_T\}$, which is very sparse.

Similar to Example 2 let $q = 5$ and $B$ be the OSLHD(5, 2) in Example 1 we can obtain an NOSLHD(125, 60) with $\rho_M = 0.1459$ and $\rho_{\text{ave}}^2 = 0.0002$.

We next provide some further properties of the $L$ constructed in (2.1). First, note that $L$ contains the center point $(0, \ldots, 0)$. If we delete the center point and properly re-scale the levels, we will obtain an LHD with $q^d - 1$ runs. Theorem 2 provides an upper bound for the pairwise column correlations of this resulting design.

**Definition 1.** The sign matrix of an $n \times m$ matrix $X = (x_{ij})$ is an $n \times m$ matrix $S_X = (s_{ij})$ with

$$s_{ij} = \begin{cases} 1, & \text{if } x_{ij} > 0; \\ 0, & \text{if } x_{ij} = 0; \\ -1, & \text{if } x_{ij} < 0. \end{cases}$$

**Theorem 2.** Suppose $L$ is the symmetric LHD($q^d, bdp$) constructed in (2.1) with $p = 1$, and $L_0$ is the matrix obtained by deleting the center point $(0, \ldots, 0)$ of $(L - S_L/2)$. If $\rho_M(T_d) \leq (q^{d-1} - 1)(q + 1)/(q(q^d + 1))$, then $L_0$ is a symmetric LHD($q^d - 1, bdp$) with

$$\rho_M(L_0) \leq \frac{\rho_M(T_d)(q^d + 1)}{q^d - 2} + \frac{3(q + 1)}{q^2(q^d - 2)} + \frac{3}{q^d(q^d - 2)}. \quad (4.1)$$
For $d = 2^c$ and $T_d$ defined in (3.1), $\rho_M(T_d) = 0$ and (4.1) reduces to
\[
\rho_M(L_0) \leq \frac{3(q + 1)}{q^2(q^d - 2)} + \frac{3}{q^d(q^d - 2)}.
\]

(4.2)
The upper bound in (4.2) decreases fast as $q$ and $d$ increase. The actual value of $\rho_M(L_0)$ is typically much smaller, as will be seen in Section 5. If $T_d$ is not column-orthogonal, the upper bound in (4.1) mainly depends on $\rho_M(T_d)$. This is consistent with the fact that $\rho_M(L)$ also depends on $\rho_M(T_d)$. When constructing $L$, we will try to minimize $\rho_M(T_d)$, so that the upper bound in (4.1) will also be small.

Note that in Theorem 2 we only derive result for $p = 1$. For $p > 1$, we can still construct NOSLHDs with the same method. It is obvious that the resulting designs are symmetric, and as will be seen in Section 5, they all have small correlations between any two distinct columns.

Let $1_m$ denote an $m \times 1$ vector with all entries unity. The following theorem offers another property of the $L$ constructed in (2.1).

**Theorem 3.** Suppose $L$ is the symmetric LHD$(q^d, bdp)$ constructed in (2.1) with $p = 1$, $m = bd$, $L_1 = ((L + S_L)^T, 1_m, -1_m)^T$, and $L_2$ is the matrix obtained by deleting the center point $(0, \ldots, 0)$ of $((L + S_L/2)^T, \frac{1}{2}1_m, -\frac{1}{2}1_m)^T$. If $\rho_M(T_d) \leq (q^{d-1} - 1)(q + 1)/[q(q^d + 1)]$, then

(i). $L_1$ is a symmetric LHD$(q^d + 2, bdp)$ with
\[
\rho_M(L_1) \leq \frac{\rho_M(T_d)(q^d - 1)}{(q^d + 2)(q^d + 3)} + \frac{6q^{d-2}(q^d - 1)(q + 1)}{(q^d + 1)(q^d + 2)(q^d + 3)} + \frac{12}{(q^d + 2)(q^d + 3)};
\]

(ii). $L_2$ is a symmetric LHD$(q^d + 1, bdp)$ with
\[
\rho_M(L_2) \leq \frac{\rho_M(T_d)(q^d - 1)}{q^d + 2} + \frac{3(q^d - 1)(q + 1)}{q^2(q^d + 1)(q^d + 2)} + \frac{3}{q^d(q^d + 2)}.
\]

(4.3)

(4.4)

Based on Theorem 3, symmetric LHDs with $q^d + 1$ or $q^d + 2$ runs can be constructed, with upper bounds of pairwise column correlations given in (4.3) and (4.4), respectively. For $d = 2^c$, if $T_d$ is defined in (3.1), then $\rho_M(T_d) = 0$ and the first items in the two upper bounds vanish, making the two bounds decrease fast as $q$ and $d$ increase.
5. Comparisons and Results

Some comparisons between the proposed approaches and some existing construction methods for OSLHDs and NOSLHDs are provided in Table 5. For simplicity, we denote the methods of Ye (1998), Cioppa and Lucas (2007), Sun, Liu, and Lin (2009, 2010), Yang and Liu (2012), Georgiou and Stylianou (2011), Georgiou and Efthimiou (2014) and the proposed methods by Ye, CL, SLL, YL, GS, GE and PM, respectively. The third column of Table 5 is the maximal possible number of factors of the LHD constructed by the corresponding method. From Table 5, it is clear that the resulting LHDs of GS and GE can only study 32 or less factors; YL has a more flexible choice of number of runs than the other methods except PM, and PM produces LHDs with almost different run sizes from that of YL. Thus the proposed methods are able to produce many new designs with flexible run sizes to accommodate more factors.

Some selected symmetric LHDs obtained by the proposed methods are listed in Table 6. Note that OSLHD(24, 12), OSLHD(25, 12), OSLHD(48, 24), and OSLHD(49, 24)
Table 6: Some selected orthogonal and nearly orthogonal symmetric LHD\((n, m)\)'s obtained by the proposed methods.

<table>
<thead>
<tr>
<th>q</th>
<th>d</th>
<th>p</th>
<th>(n = q^d + i), ((i = -1, 0, 1, \text{or } 2))</th>
<th>(m = bdp)</th>
<th>(\rho^k_M)</th>
<th>(\rho_M)</th>
<th>(\rho_{\text{ave}})</th>
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<td>0.3205</td>
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<td>264</td>
<td>0.1859</td>
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</table>
have been constructed by Georgiou and Efthimiou (2014) thus are not included in Table 6. All designs in the table can accommodate factors up to half of the run sizes. The OSLHD(81, 40), OSLHD(625, 312) and OSLHD(289, 144) listed in the table are all new and saturated. The OSLHD(121, 36) and OSLHD(169, 42), although not saturated, are new and can also accommodate many factors. For NOSLHDs, the values of $\rho_M$ and $\rho^2_{ave}$ are offered. As a comparison, for each combination $(n, m)$, the average of the $\rho_M$ values of 1000 randomly generated LHD($n, m$)'s, denoted by $\rho^R_M$, is also provided in Table 6. It is clear that most NOSLHDs in the table have much smaller $\rho_M$'s than their corresponding randomly generated LHDs. For NOSLHDs with 80, 82, 83, 288, 290, 291, 624, 626, and 627 runs, the $\rho_M$'s are less than (or around) 0.01. These designs are actually very close to OSLHDs, only with tiny correlations between few pairs of columns. Such designs are obviously very useful for computer experiments and have never been constructed by existing methods. The $\rho_M$ values of other NOSLHDs are all less than (or around) 0.1 except for the ones generated from $q = 3$ and $d = 3$, and $q = 5$ and $d = 3$. Their $\rho_M$'s are around 0.15. However, all of them have very small $\rho^2_{ave}$'s. This implies that nonzero correlations exist only between few pairs of columns for the designs. Thus they are ideal for computer experiments.

6. Concluding Remarks

LHDs have been popular for computer experiments. Orthogonal LHDs ensure uncorrected estimates of linear effects when a first-order model is fitted. However, if second-order effects are nonnegligible, a symmetric LHD is preferred. A symmetric LHD is able to estimate the linear effects without being correlated with the estimates of second-order effects. In this paper, we propose some methods to construct OSLHDs and NOSLHDs. The resulting OSLHDs have the maximum possible number of factors and are more economical than existing ones. The resulting NOSLHDs, though have low correlations among the estimates of the linear effects of all factors, are able to keep their estimates uncorrelated with all quadratic effects and bilinear interactions.

Two issues related to this research are particularly worthy of further study. The first one has something to do with the maximal number of factors. It is proved that if a
saturated OSLHD with \( q (q = 3 \text{ or } q \geq 5) \) runs is available, then the resulting OSLHD is saturated (i.e., the number of factors attains its maximal value). For NOSLHDs, the column sizes can be larger. Thus how to add columns to available LHDs as well as keeping their symmetry is an important issue to be explored. The second related issue concerns the construction of column-orthogonal designs with fewer levels than runs. Designs with many levels are desirable, but it is not essential to keep the number of runs equal to the number of levels. These designs are quite suitable for practical use, and in addition, they can be viewed as stepping stones to space-filling design as a good space-filling design must be column-orthogonal or nearly so (Bingham, Sitter, and Tang (2009); Sun, Pang, and Liu (2011); Georgiou, Koukouvinos, and Liu (2014); Yuan, Lin, and Liu (2017)).

Acknowledgements
The authors thank Editor Ruey S. Tsay, an associate editor, and two referees for their valuable comments and suggestions. This work was supported by the National Natural Science Foundation of China (Grant Nos. 11431006 and 11471069), the Specialized Research Fund for the Doctoral Program of Higher Education of China (Grant No. 20130031110002), the “131” Talents Program of Tianjin, Project 613319 and National Security Agency (Grant No. H98230-15-1-0253). The first two authors contribute equally to this work.

Appendix: Proof of Theorems

The following two lemmas will be used for proving Theorem 2.

**Lemma A.1.** Let \( A = (a_{ij})_{q^d \times d} \) be a \( q^d \) full factorial design with levels \( k - (q + 1)/2 \) for \( k = 1, \ldots, q \) where \( q \) is an odd prime, and \( L = AT_d \). Then

\[
A^T S_L = -\frac{q^2 - 1}{4} T_d.
\]

**Lemma A.2.** Let \( A_1 \) and \( A_2 \) be two \( q^d \) full factorial designs with levels \( k - (q + 1)/2 \) for \( k = 1, \ldots, q \) where \( q \) is an odd prime, and \( L_1 = A_1 T_d \). Suppose any column of \( A_1 \) is orthogonal to any column of \( A_2 \), that is, all possible level combinations for
the two columns appear equally often. Then each element of $A_2^T S_{L_1}$, say $(A_2^T S_{L_1})_{i,j}$, $i, j = 1, \ldots, d$, satisfies that

$$\left| (A_2^T S_{L_1})_{i,j} \right| \leq \frac{q^{d-2}(q^2 - 1)}{4}.$$ 

A.1. Proof of Lemma [A.1]

For a given $j$, $j \in \{1, \ldots, d\}$, let $\{\pi_1^j, \pi_2^j, \ldots, \pi_d^j\}$ be the row index of $\{q^{d-1}, q^{d-2}, \ldots, q, 1\}$ (up to sign changes) in the $j$th column of $T_d$. Without loss of generality, suppose the last row of $A$ is the center point $(0, 0, \ldots, 0)$. For any $i, i \in \{1, \ldots, q^d - 1\}$, let $p = p(i, j)$ satisfy that $(S_A)_{i, \pi_i^j} = \cdots = (S_A)_{i, \pi_{p-1}^j} = 0$ and $(S_A)_{i, \pi_p^j} \neq 0$, $p \leq d$. Then $(S_L)_{i,j} = (S_A)_{i, \pi_p^j}(S_{T_d})_{\pi_p^j,j}$. Hence,

$$(A^T S_L)_{ij} = \sum_{l=1}^{q^{d-1}} a_l(S_A)_{i,\pi_l^j}(S_{T_d})_{\pi_l^j,j}, \text{ for } l, j = 1, \ldots, d. \quad (A.1)$$

Note that for the $j$th column of the design $A$, $q^{d-1}(q - 1)$ rows have $p(i, j) = 1$, $q^{d-2}(q - 1)$ rows have $p(i, j) = 2$, $\ldots$ $q - 1$ rows have $p(i, j) = d$. Denote $E_h^j = \{i : p(i, j) = h\}$ for $h = 1, \ldots, d$. Then from (A.1),

$$(A^T S_L)_{ij} = \sum_{h=1}^{d} (S_{T_d})_{\pi_h^j,j} \sum_{i \in E_h^j} a_i(S_A)_{i,\pi_i^j}. \quad (A.2)$$

For $\pi_h^j = l$, $\sum_{i \in E_h^j} a_i(S_A)_{i,\pi_i^j} = \sum_{i \in E_h^j} a_i = 2q^{d-h} \sum_{k=1}^{(q-1)/2} k = q^{d-h}(q^2 - 1)/4$. For $\pi_h^j \neq l$, suppose $l = \pi_h^j$ where $h \in \{1, \ldots, d\}$ and $h \neq h$. If $h < h$, $a_i = 0$ for all $i \in E_h^j$. If $h > h$, in the rows $i \in E_h^j$ where the levels of the $\pi_h^j$th column of $A$ are equal, the levels of the $h$th column occur equally often. Therefore, for $\pi_h^j \neq l$, $\sum_{i \in E_h^j} a_i(S_A)_{i,\pi_i^j} = 0$. Then from (A.2), for $h = 1, \ldots, d$,

$$(A^T S_L)_{\pi_h^j, j} = \frac{q^{d-h}(q^2 - 1)}{4} (S_{T_d})_{\pi_h^j, j} = \frac{q^2 - 1}{4} (T_d)_{\pi_h^j, j}.$$

This completes the proof.

A.2. Proof of Lemma [A.2]

Denote $A_2 = (a_{ij})$. For a given $j$, $j \in \{1, \ldots, d\}$, let $\{\pi_1^j, \pi_2^j, \ldots, \pi_d^j\}$ be the row index of $\{q^{d-1}, q^{d-2}, \ldots, q, 1\}$ (up to sign changes) in the $j$th column of $T_d$. Without
loss of generality, suppose the last row of $A_1$ is the center point $(0, 0, \ldots, 0)$. For any $i$, $i \in \{1, \ldots, q^d - 1\}$, let $p = p(i, j)$ satisfy that $(S_{A_1})_{i,\pi_1^i} = \cdots = (S_{A_1})_{i,\pi_{p-1}^i} = 0$ and $(S_{A_1})_{i,\pi_p^i} \neq 0$, $p \leq d$. Then $(S_{L_1})_{i,j} = (S_{A_1})_{i,\pi_p^i}(S_{T_d})_{\pi_p^i,j}$, and

$$
(A_2^T S_{L_1})_{ij} = \sum_{i=1}^{q^d-1} a_{il}(S_{A_1})_{i,\pi_p^i}(S_{T_d})_{\pi_p^i,j}, \text{ for } l, j = 1, \ldots, d.
$$

(A.3)

Note that for the $j$th column of the design $A_1$, $q^{d-1}(q - 1)$ rows have $p(i, j) = 1$, $q^{d-2}(q - 1)$ rows have $p(i, j) = 2$, $\ldots$, $q - 1$ rows have $p(i, j) = d$. Denote $E_h^j = \{i : p(i, j) = h\}$ for $h = 1, \ldots, d$. Then from (A.3),

$$
(A_2^T S_{L_1})_{ij} = \sum_{h=1}^{d} \sum_{i \in E_h^j} a_{il}(S_{A_1})_{i,\pi_p^i}.
$$

(A.4)

As for $i \notin E_1^j$, $(S_{A_1})_{i,\pi_1^i} = 0$, and any column of $A_1$ is orthogonal to any column of $A_2$, $\sum_{i \in E_1^j} a_{il}(S_{A_1})_{i,\pi_1} = \sum_{i=1}^{q^d} a_{il}(S_{A_1})_{i,\pi_1^i} = 0$. From (A.4), for $l, j = 1, \ldots, d$,

$$
|A_{2}^{T} S_{L_{1}}|_{ij} = \left| \sum_{h=2}^{d} \sum_{i \in E_h^j} a_{il}(S_{A_1})_{i,\pi_p^i} \right| \leq \sum_{h=2}^{d} \sum_{i \in E_h^j} |a_{il}|.
$$

The result follows from the fact that $\sum_{h=2}^{d} \sum_{i \in E_h^j} |a_{il}| = \sum_{i \notin E_1^j} |a_{il}| = q^{d-2} \left( 2 \sum_{k=1}^{(q-1)/2} k \right) = q^{d-2}(q^2 - 1)/4.$

A.3. Proof of Theorem 1

For Part (i), the assertion that $L$ is an LHD($n, mp$) with levels $\{- (n - 1)/2, -(n - 3)/2, \ldots, (n - 1)/2\}$ follows from Pang, Liu, and Lin (2009). For the symmetry of $L$, we need to show that $\hat{D} = (\hat{D}^{(1)}, \ldots, D^{(p)})$ is symmetric, i.e., for any row $d_i$ of $\hat{D}$, $i = 1, \ldots, n$, $-d_i$ is also one of its rows. Denote the $i$th row of $D$ as $(a_{i1}, \ldots, a_{im})$ for $i = 1, \ldots, n$, then $d_i = (b_{c_{i1,1}}, \ldots, b_{c_{im,1}}, \ldots, b_{c_{i1,p}}, \ldots, b_{c_{im,p}})$, where $c_{ik} = (q+1)/2 + a_{ik}$ (mod $q$) for $k = 1, \ldots, m$. If $(a_{i1}, \ldots, a_{im}) = (0, \ldots, 0)$, notice that $b_{(q+1)/2,j} = 0$ for $j = 1, \ldots, p$, then $d_i = (0, \ldots, 0)$. If $(a_{i1}, \ldots, a_{im}) \neq (0, \ldots, 0)$, since $D$ is a regular design, $(q - a_{i1}, \ldots, q - a_{im})$ (mod $q$) is also its row, say the $l$th row. Then the $l$th row of $\hat{D}$ is $d_l = (b_{c_{i1,1}}, \ldots, b_{c_{im,1}}, \ldots, b_{c_{i1,p}}, \ldots, b_{c_{im,p}})$ where $c_{lk} = (q+1)/2 - a_{ik}$ (mod $q$) for $k = 1, \ldots, m$. Then $b_{c_{ik,j}} = -b_{c_{ik,j}}$ for $j = 1, \ldots, p$ and $k = 1, \ldots, m$, and $d_l = -d_i$. 
For Part (ii), we have

\[ C_L = 12L^T L / (n(n^2 - 1)). \] (A.5)

Since \( L^{(k)} = D^{(k)}(I_b \otimes T_d) \), thus \( L^{(k)T} L^{(j)} = (I_b \otimes T_d)^T D^{(k)T} D^{(j)}(I_b \otimes T_d) \). It follows from the proof of Theorem 1 in Lin, Mukerjee, and Tang (2009) that \( D^{(k)T} D^{(j)} = n(q^2 - 1)c_{kj} I_{bd} / 12 \), for \( k, j = 1, \ldots, p \), where \( c_{kj} \) is the \((k, j)\)th element of \( C_B = 12B^T B / (q(q^2 - 1)) \). Then \( L^T L = n(n^2 - 1)C_B \otimes I_b \otimes C_{T_d} / 12 \). Part (ii) is now proved from (A.5).

### A.4. Proof of Theorem 2

It is obvious that \( L_0 \) is a symmetric LHD. From the definition of \( L_0 \),

\[ L_0^T L_0 = (L - \frac{1}{2} S_L)^T (L - \frac{1}{2} S_L) = L^T L - \frac{1}{2} L^T S_L - \frac{1}{2} S_L^T L + \frac{1}{4} S_L^T S_L. \] (A.6)

Firstly, for \( L^T L \), by Corollary 2,

\[ (L^T L)_{ij} \leq \rho_M(T_d) q^d(q^{2d} - 1) / 12 \text{ for } i \neq j. \] (A.7)

Denote \( D^{(1)} = (A_1, \ldots, A_b) \) and \( L_i = A_i T_d \), where each \( A_i \) is a full factorial design with levels \( k - (q + 1)/2 \) for \( k = 1, \ldots, q \), \( i = 1, \ldots, b \). For the second item of (A.6),

\[ L^T S_L = \text{diag}\{T_d^T, \ldots, T_d^T\}(A_1, \ldots, A_b)^T (S_{L_1}, \ldots, S_{L_b}) \]

\[ = \begin{pmatrix} T_d^T A_1^T S_{L_1} & T_d^T A_1^T S_{L_2} & \cdots & T_d^T A_1^T S_{L_b} \\ \vdots & \vdots & \ddots & \vdots \\ T_d^T A_b^T S_{L_1} & T_d^T A_b^T S_{L_2} & \cdots & T_d^T A_b^T S_{L_b} \end{pmatrix}. \]

For diagonal block, from Lemma A.1

\[ T_d^T A_k^T S_{L_k} = \frac{q^2 - 1}{4} T_d^T T_d \text{ for } k = 1, \ldots, b. \]

Hence,

\[ |(T_d^T A_k^T S_{L_k})_{ij}| \leq \frac{q^{2d} - 1}{4} \rho_M(T_d). \] (A.8)
For the off-diagonal block, by Lemma A.2, for $k \neq l$ and $i, j = 1, \ldots, d$,
\[
| (T_d^T A_k^T S_L)_{ij} | \leq \frac{q^{d-2}(q^2 - 1)}{4} \left( 1 + q + \ldots + q^{d-1} \right) = \frac{q^{d-2}(q + 1)(q^d - 1)}{4} \quad (A.9)
\]
For $\rho_M(T_d) \leq q^{d-2}(q + 1)/(q^d + 1)$, the bound in (A.8) is no more than that in (A.9).
For the forth item of (A.6), it is obvious that for $i, j = 1, \ldots, bd$,
\[
(S_L^T S_L)_{i,j} \leq q^d - 1 \quad (A.10)
\]
From (A.7), (A.8), (A.9) and (A.10), we have
\[
\rho_M(L_0) \leq \frac{\rho_M(T_d) q^d(2q^2 - 1)/12 + q^{d-2}(q + 1)(q^d - 1)/4 + (q^d - 1)/4}{q^d(q^2 - 1)/12 - (q^{2d} - 1)/4 + (q^d - 1)/4} = \frac{\rho_M(T_d)(q^d + 1)}{q^d - 2} + \frac{3(q + 1)}{q^2(q^d - 2)} + \frac{3}{q^d(q^d - 2)}.
\]

A.5. Proof of Theorem 3

(i). It is obvious that $L_1$ is a symmetric LHD. Consider the value of $\rho_{ij}(L_1)$ for $i \neq j$. Since
\[
L_1^T L_1 = ((L + S_L)^T, 1, -1, 1, -1)^T((L + S_L)^T, 1, -1, 1, -1)^T
\]
\[
= L^T L + L^T S_L + S_L^T L + S_L^T S_L + 2 \cdot 1^T m 1^T m
\]
From (A.7), (A.8), (A.9) and (A.10), we have
\[
\rho_M(L_1) \leq \frac{\rho_M(T_d) q^d(2q^2 - 1)/12 + q^{d-2}(q + 1)(q^d - 1)/2 + (q^d - 1) + 2}{q^d(q^2 - 1)/12 + (q^{2d} - 1)/2 + (q^d - 1) + 2} = \frac{\rho_M(T_d) q^d(q^d - 1)}{(q^d + 2)(q^d + 3)} + \frac{6q^{d-2}(q^d - 1)(q + 1)}{(q^d + 1)(q^d + 2)(q^d + 3)} + \frac{12}{(q^d + 2)(q^d + 3)}.
\]
The proof of (ii) is similar to that of (i) and is thus omitted.

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