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CONSTRUCTION OF ORTHOGONAL SYMMETRIC LATIN HYPERCUBE DESIGNS

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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. Several methods for constructing nearly orthogonal symmetric LHDs are also provided. The constructed orthogonal and nearly orthogonal LHDs can 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 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 are present because the estimates of linear main effects may be biased by nonnegligible second-order effects. This paper constructs orthogonal symmetric LHDs (OSLHDs) that 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) symmetric LHDs are proposed. In particular, the resulting OSLHDs can 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. 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 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. 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 $GF(q)[x] = \{a_0 + a_1x + \cdots + a_{d-1}x^{d-1}, a_0, \ldots, a_d \in GF(q)\}$. A q^d-run full factorial design has d columns $\mathbf{1}, \ldots, \boldsymbol{d}$. Each column, or a generated column, of $\mathbf{1}, \ldots, \boldsymbol{d}$, can be denoted by $\mathbf{1}^{a_0} \cdots \boldsymbol{d}^{a_{d-1}}$ for some $a_0, \ldots, a_d \in GF(q)$ and corresponds to a nonzero element $a_0 + a_1x + \cdots + a_{d-1}x^{d-1}$ in $GF(q)[x]$. 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 $b = \lfloor (q^d - 1)/(d(q-1)) \rfloor$, 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 a 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 $b_{(q+1)/2,j}, \ldots, b_{qj}, b_{1j}, \ldots, b_{(q-1)/2,j}$, 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 $T = \mathrm{diag}\{T_d, \ldots, T_d\}$ with T_d repeating b times.

Step 5. The resulting design matrix is then

$$L = (L^{(1)}, \ldots, L^{(p)}). \tag{2.1}$$

For any matrix $X = (x_1, \ldots, x_m)$ where x_i is the ith column of X for $i =$

Table 1. The regular design D (in transpose) in Example 1.

0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4
0	0	0	0	0	1	1	1	1	1	2	2	2	2	2	3	3	3	3	3	4	4	4	4	4
3	1	4	2	0	2	0	3	1	4	1	4	2	0	3	0	3	1	4	2	4	2	0	3	1
0	2	4	1	3	4	1	3	0	2	3	0	2	4	1	2	4	1	3	0	1	3	0	2	4
2	4	1	3	0	0	2	4	1	3	3	0	2	4	1	1	3	0	2	4	4	1	3	0	2
1	0	4	3	2	0	4	3	2	1	4	3	2	1	0	3	2	1	0	4	2	1	0	4	3

$1, \ldots, m$, define $\rho_{ij}(X) = x_i^{\mathrm{T}} x_j / (x_i^{\mathrm{T}} x_i x_j^{\mathrm{T}} x_j)^{1/2}$ as the correlation between the ith and jth 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) with

$$B = \begin{pmatrix} -2 & -1 & 0 & 1 & 2 \\ -1 & 2 & 0 & -2 & 1 \end{pmatrix}^{\mathrm{T}}.$$

Then $D^{(1)}$ and $D^{(2)}$ can be obtained by replacing the levels $0, \ldots, 4$ of D with the entries in the first and second column of B, respectively, following the replacement rule specified in Step 3 of Algorithm 1. Let

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

and $L^{(k)} = D^{(k)} T$ with $T = \mathrm{diag}\{T_2, T_2, T_2\}$, for $k = 1, 2$. Then it can be easily checked that $L = (L^{(1)}, L^{(2)})$, shown in Table 2, is an OSLHD$(25, 12)$.

Example 1 is a typical illustration for constructing an OSLHD from the proposed algorithm.

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

−12	−7	−2	3	8	−11	−6	−1	4	9	−10	−5	0	5	10	−9	−4	1	6	11	−8	−3	2	7	12
−8	−9	−10	−11	−12	−3	−4	−5	−6	−7	2	1	0	−1	−2	7	6	5	4	3	12	11	10	9	8
3	−5	12	−1	−9	2	−11	6	−7	10	−4	8	0	−8	4	−10	7	−6	11	−2	9	1	−12	5	−3
−11	1	8	−5	7	10	−3	4	−9	−2	6	−12	0	12	−6	2	9	−4	3	−10	−7	5	−8	−1	11
−1	8	−3	6	−10	−12	2	11	−5	4	7	−9	0	9	−7	−4	5	−11	−2	12	10	−6	3	−8	1
−5	−12	11	4	2	−8	10	3	1	−6	9	7	0	−7	−9	6	−1	−3	−10	8	−2	−4	−11	12	5
−6	9	−1	−11	4	−3	12	2	−8	7	−5	10	0	−10	5	−7	8	−2	−12	3	−4	11	1	−9	6
−4	−7	−5	−3	−6	11	8	10	12	9	1	−2	0	2	−1	−9	−12	−10	−8	−11	6	3	5	7	4
−11	10	6	2	−7	1	−3	−12	9	5	8	4	0	−4	−8	−5	−9	12	3	−1	7	−2	−6	−10	11
−3	−2	4	10	−9	5	11	−8	−7	−1	−12	−6	0	6	12	1	7	8	−11	−5	9	−10	−4	2	3
2	4	11	−12	−5	−6	1	3	10	−8	−9	−7	0	7	9	8	−10	−3	−1	6	5	12	−11	−4	−2
10	−6	3	−8	1	−4	5	−11	−2	12	7	−9	0	9	−7	−12	2	11	−5	4	−1	8	−3	6	−10

Remark 1. 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). 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

Corollary 1. *If B is orthogonal and T_d is column-orthogonal, $T_d^T T_d = a_d I_d$ 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

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

Here $(q^d - 1)/(d(q-1))$ 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$(81, 40)$. An OSLHD(n, m) is second-order orthogonal, satisfying $m \le \lfloor n/2 \rfloor$ (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*

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

OLHD$(11,3)$												
−5	−4	−3	−2	−1	0	1	2	3	4	5		
−5	3	1	4	2	0	−2	−4	−1	−3	5		
1	2	−5	3	−4	0	4	−3	5	−2	−1		
OLHD$(13,3)$												
−6	−5	−4	−3	−2	−1	0	1	2	3	4	5	6
−6	5	4	−2	−1	3	0	−3	1	2	−4	−5	6
1	3	−6	2	−4	5	0	−5	4	−2	6	−3	−1

constructed in (2.1) *is saturated.*

For $q \geq 5$, if B is saturated, 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 1 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; they were 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.

4. Construction of NOSLHDs

For given q and p, if there does not exist an 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 $\rho^2_{\text{ave}}(X) = \sum_{i<j} \rho^2_{ij}(X)/(m(m-1)/2)$. The ρ_M measures the maximum correlation, and the ρ^2_{ave} measures both magnitudes and sparsity of the correlations. A result from Theorem 1 gives the values for ρ_M and ρ^2_{ave} of the resulting design L in (2.1).

Corollary 2. *For L in* (2.1)*, we have*

$\rho_M(L) = \max\{\rho_M(B), \rho_M(T_d)\}$, *and*

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
2	0	0	0	1	1	1	2	2	2	0	0	0	1	1	1	2	2	2	0	0	0	1	1	1	2	2	2
3	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2	2
$\mathbf{1}^2\mathbf{2}$	0	2	1	1	0	2	2	1	0	0	2	1	1	0	2	2	1	0	0	2	1	1	0	2	2	1	0
$\mathbf{2}^2\mathbf{3}$	0	0	0	2	2	2	1	1	1	1	1	1	0	0	0	2	2	2	2	2	2	1	1	1	0	0	0
$\mathbf{1}^2\mathbf{2}\mathbf{3}^2$	0	2	1	1	0	2	2	1	0	2	1	0	0	2	1	1	0	2	1	0	2	2	1	0	0	2	1
123	0	1	2	1	2	0	2	0	1	1	2	0	2	0	1	0	1	2	2	0	1	0	1	2	1	2	0
$\mathbf{1}^2\mathbf{2}^2\mathbf{3}$	0	2	1	2	1	0	1	0	2	1	0	2	0	2	1	2	1	0	2	1	0	1	0	2	0	2	1
$\mathbf{1}^2\mathbf{3}^2$	0	2	1	0	2	1	0	2	1	2	1	0	2	1	0	2	1	0	1	0	2	1	0	2	1	0	2
12	0	1	2	1	2	0	2	0	1	0	1	2	1	2	0	2	0	1	0	1	2	1	2	0	2	0	1
23	0	0	0	1	1	1	2	2	2	1	1	1	2	2	2	0	0	0	2	2	2	0	0	0	1	1	1
$\mathbf{1}^2\mathbf{2}\mathbf{3}$	0	2	1	1	0	2	2	1	0	1	0	2	2	1	0	0	2	1	2	1	0	0	2	1	1	0	2

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

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 $\rho_{\text{ave}}^2 = 0.0003$, 0.0002, 0.0001, and 0.0001, respectively.

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 ρ_M and ρ_{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 three consecutive columns of D form a full factorial design. Let $B = (-1, 0, 1)^{\mathrm{T}}$,

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

with correlation matrix

$$C_T = \begin{pmatrix} 1 & 0.0110 & -0.1648 \\ 0.0110 & 1 & -0.0989 \\ -0.1648 & -0.0989 & 1 \end{pmatrix},$$

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 $\rho^2_{\text{ave}}(L) = 0.0022$. 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 $\rho^2_{\text{ave}} = 0.0002$.

We next provide some further properties of the L constructed in (2.1). First, L contains the center point $(0, \ldots, 0)$. If we delete the center point and properly re-scale the levels, we obtain an LHD with $q^d - 1$ runs. Theorem 2 provides an upper bound for the pairwise column correlations of the 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 $\rho_M(T_d) \le (q^{d-1} - 1)(q + 1)/[q(q^d + 1)]$, then L_0 is a symmetric LHD$(q^d - 1, bdp)$ with*

$$\rho_M(L_0) \le \frac{\rho_M(T_d)(q^d + 1)}{q^d - 2} + \frac{3(q + 1)}{q^2(q^d - 2)} + \frac{3}{q^d(q^d - 2)}. \tag{4.1}$$

For $d = 2^c$ and T_d defined in (3.1), $\rho_M(T_d) = 0$ and (4.1) reduces to

$$\rho_M(L_0) \le \frac{3(q + 1)}{q^2(q^d - 2)} + \frac{3}{q^d(q^d - 2)}. \tag{4.2}$$

The upper bound in (4.2) decreases quickly as q and d increase. The 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 try to minimize $\rho_M(T_d)$, so that the upper bound in (4.1) is also small.

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 distinct columns.

Let 1_m denote an $m \times 1$ vector with all entries unity. We have 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 $p = 1$, $m = bd$, $L_1 = ((L + S_L)^{\mathrm{T}}, 1_m, -1_m)^{\mathrm{T}}$, and L_2 is the matrix obtained by deleting the center point $(0, \ldots, 0)$ of $((L + S_L/2)^{\mathrm{T}}, 1/21_m, -1/21_m)^{\mathrm{T}}$. 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*

$$\rho_M(L_1) \leq \frac{\rho_M(T_d)q^d(q^d-1)}{(q^d + 2)(q^d + 3)} + \frac{6q^{d-2}(q^d - 1)(q + 1)}{(q^d+1)(q^d+2)(q^d+3)} + \frac{12}{(q^d+2)(q^d+3)}; \quad (4.3)$$

(ii). *L_2 is a symmetric LHD$(q^d + 1, bdp)$ with*

$$\rho_M(L_2) \leq \frac{\rho_M(T_d)(q^d - 1)}{q^d + 2} + \frac{3(q^d - 1)(q + 1)}{q^2(q^d + 1)(q^d + 2)} + \frac{3}{q^d(q^d + 2)}. \quad (4.4)$$

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 quickly as q and d increase.

5. Comparisons and Results

Some comparisons between the proposed approaches and 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 that 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

Table 5. Some existing results of OSLHDs and NOSLHDs.

Method	Run size n	Maximal number of factors	OSLHD or NOSLHD
Ye	2^{r+1} or $2^{r+1}+1$	$2r$	OSLHD
CL	2^{r+1} or $2^{r+1}+1$	$1+r+\binom{r}{2}$	OSLHD
SLL	$c2^{r+1}$ or $c2^{r+1}+1$	2^r	OSLHD
YL	$c2^{r+1}$ or $c2^{r+1}+1$	2^r	OSLHD
	$c2^{r+1}+2$ or $c2^{r+1}+3$	2^r	NOSLHD
GS	7	3	NOSLHD
	$8k$ or $8k+1$	$4k(k=1,2,\ldots,6,8)$	OSLHD
	$8k+2$	$4k(k=1,2,\ldots,6,8)$	NOSLHD
	$8k+3$	$4k(k=1,2,\ldots,6)$	NOSLHD
GE	$2ar$ or $2ar+1$	$a=12,16,20,24$	OSLHD
PM	q^d	$pd\left\lfloor\dfrac{q^d-1}{(q-1)d}\right\rfloor$	OSLHD and NOSLHD†
	q^d-1, q^d+1 or q^d+2	$pd\left\lfloor\dfrac{q^d-1}{(q-1)d}\right\rfloor$	NOSLHD

†: OSLHD can be obtained when $d=2^c$ and an OSLHD(q,p) exists; for otherwise, only NOSLHD is possible.

OSLHD(49, 24) have been constructed by Georgiou and Efthimiou (2014) and 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 ρ_M and ρ^2_{ave} are offered. As a comparison, for each combination (n,m), the average of the ρ_M values of 1,000 randomly generated LHD(n,m)'s, denoted by ρ_M^R, is also provided in Table 6. It is clear that most NOSLHDs in the table have much smaller ρ_M's than their corresponding randomly generated LHDs. For NOSLHDs with 80, 82, 83, 288, 290, 291, 624, 626, and 627 runs, the ρ_M's are less than (or around) 0.01. These designs are very close to OSLHDs, with only tiny correlations between few pairs of columns. Such designs are obviously useful for computer experiments and have never been constructed by existing methods. The ρ_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 ρ_M's are around 0.15. All of them have very small ρ^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.

Table 6. Some selected orthogonal and nearly orthogonal symmetric LHD(n, m)'s obtained by the proposed methods.

q	d	p	$n = q^d + i$, ($i = -1, 0, 1$, or 2)	$m = bdp$	ρ_M^R	ρ_M	ρ^2_{ave}
3	3	1	26	12	0.5049	0.1644	0.0019
			27	12	0.4952	0.1648	0.0022
			28	12	0.4971	0.1642	0.0030
			29	12	0.4762	0.1626	0.0042
3	4	1	80	40	0.3727	0.0083	0.0000
			81	40			
			82	40	0.3748	0.0079	0.0000
			83	40	0.3615	0.0156	0.0000
5	2	2	26	12	0.5049	0.0236	0.0001
			27	12	0.4952	0.0452	0.0005
5	3	2	124	60	0.3205	0.1459	0.0002
			125	60	0.3210	0.1459	0.0003
			126	60	0.3206	0.1459	0.0003
			127	60	0.3234	0.1459	0.0003
5	4	2	624	312	0.1748	0.0005	0.0000
			625	312			
			626	312	0.1730	0.0005	0.0000
			627	312	0.1736	0.0010	0.0000
7	2	3	50	24	0.4355	0.0573	0.0006
			51	24	0.4265	0.0440	0.0004
11	2	3	121	36			
11	2	5	120	60	0.3290	0.0949	0.0003
			121	60	0.3231	0.0909	0.0003
			122	60	0.3220	0.0870	0.0003
			123	60	0.3264	0.0833	0.0003
13	2	3	169	42			
13	2	6	168	84	0.2862	0.1032	0.0003
			169	84	0.2889	0.0989	0.0002
			170	84	0.2858	0.0946	0.0002
			171	84	0.2827	0.0904	0.0002
17	2	8	288	144	0.2354	0.0006	0.0000
			289	144			
			290	144	0.2346	0.0006	0.0000
			291	144	0.2319	0.0012	0.0000
19	2	9	361	180	0.2186	0.1053	0.0001
23	2	11	529	264	0.1859	0.1067	0.0001

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. 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 they 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 has something to do with the maximal number of factors. It is proved that if a saturated OSLHD with q ($q = 3$ 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)).

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Appendix: Proofs of Theorems

Lemma 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*

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

Lemma 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 $L_1 = A_1T_d$. If any column of A_1 is orthogonal to any column of A_2, then each element of $A_2^{\mathrm{T}}S_{L_1}$, say $\left(A_2^{\mathrm{T}}S_{L_1}\right)_{i,j}$, $i,j=1,\ldots,d$, satisfies*

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

A.1. Proof of Lemma 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 jth 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 $(S_A)_{i,\pi_1^j}=\cdots=(S_A)_{i,\pi_{p-1}^j}=0$ and $(S_A)_{i,\pi_p^j}\neq 0$, $p\le d$. Then $(S_L)_{i,j}=(S_A)_{i,\pi_p^j}(S_{T_d})_{\pi_p^j,j}$. Hence,

$$(A^{\mathrm{T}}S_L)_{lj} = \sum_{i=1}^{q^d-1} a_{il}(S_A)_{i,\pi_p^j}(S_{T_d})_{\pi_p^j,j}, \text{ for } l,j=1,\ldots,d. \tag{A.1}$$

Here for the jth 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 $p(i,j)=d$. Let $E_h^j=\{i: p(i,j)=h\}$ for $h=1,\ldots,d$. Then from (A.1),

$$(A^{\mathrm{T}}S_L)_{lj} = \sum_{h=1}^{d}(S_{T_d})_{\pi_h^j,j}\sum_{i\in E_h^j} a_{il}(S_A)_{i,\pi_h^j}. \tag{A.2}$$

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

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

This completes the proof.

A.2. Proof of Lemma 2

Let $A_2=(a_{ij})$. 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 jth 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 $(S_{A_1})_{i,\pi_1^j} = \cdots = (S_{A_1})_{i,\pi_{p-1}^j} = 0$ and $(S_{A_1})_{i,\pi_p^j} \neq 0$, $p \leq d$. Then $(S_{L_1})_{i,j} = (S_{A_1})_{i,\pi_p^j}(S_{T_d})_{\pi_p^j,j}$, and

$$(A_2^{\mathrm{T}} S_{L_1})_{lj} = \sum_{i=1}^{q^d-1} a_{il}(S_{A_1})_{i,\pi_p^j}(S_{T_d})_{\pi_p^j,j}, \text{ for } l,j = 1,\ldots,d. \tag{A.3}$$

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

$$(A_2^{\mathrm{T}} S_{L_1})_{lj} = \sum_{h=1}^{d}(S_{T_d})_{\pi_h^j,j} \sum_{i \in E_h^j} a_{il}(S_{A_1})_{i,\pi_h^j}. \tag{A.4}$$

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

$$\left|(A_2^{\mathrm{T}} S_{L_1})_{lj}\right| = \left|\sum_{h=2}^{d}(S_{T_d})_{\pi_h^j,j} \sum_{i \in E_h^j} a_{il}(S_{A_1})_{i,\pi_h^j}\right| \leq \sum_{h=2}^{d}\sum_{i\in E_h^j}|a_{il}|.$$

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

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 $\tilde{D} = (D^{(1)},\ldots,D^{(p)})$ is symmetric, i.e., for any row d_i of $\tilde{D}$, $i = 1,\ldots,n$, $-d_i$ is also one of its rows. Denote the ith row of D by $(a_{i1},\ldots,a_{im})$ 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 $c_{ik} = (q+1)/2 + a_{ik} \pmod q$ 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, $(q-a_{i1},\ldots,q-a_{im}) \pmod q$ is also its row, say the lth row. Then the lth row of $\tilde{D}$ is $d_l = (b_{e_{l1},1},\ldots,b_{e_{lm},1},\ldots, b_{e_{l1},p},\ldots,b_{e_{lm},p})$ where $e_{lk} = (q+1)/2 - a_{ik} \pmod q$ for $k = 1,\ldots,m$. Then $b_{e_{lk},j} = -b_{c_{ik},j}$ for $j = 1,\ldots,p$ and $k = 1,\ldots,m$, and $d_l = -d_i$.

For Part (ii), we have

$$C_L = \frac{12L^{\mathrm{T}}L}{n(n^2-1)}. \tag{A.5}$$

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

$$L_0^{\mathrm{T}}L_0 = \left(L - \frac{1}{2}S_L\right)^{\mathrm{T}}\left(L - \frac{1}{2}S_L\right) = L^{\mathrm{T}}L - \frac{1}{2}L^{\mathrm{T}}S_L - \frac{1}{2}S_L^{\mathrm{T}}L + \frac{1}{4}S_L^{\mathrm{T}}S_L. \tag{A.6}$$

For $L^{\mathrm{T}}L$, by Corollary 2,

$$(L^{\mathrm{T}}L)_{ij} \le \frac{\rho_M(T_d)q^d(q^{2d}-1)}{12} \text{ for } i \ne j. \tag{A.7}$$

Take $D^{(1)} = (A_1,\ldots,A_b)$ and $L_i = A_iT_d$, 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),

$$L^{\mathrm{T}}S_L = \mathrm{diag}\{T_d^{\mathrm{T}},\ldots,T_d^{\mathrm{T}}\}(A_1,\ldots,A_b)^{\mathrm{T}}(S_{L_1},\ldots,S_{L_b}) = \begin{pmatrix} T_d^{\mathrm{T}}A_1^{\mathrm{T}}S_{L_1} & T_d^{\mathrm{T}}A_1^{\mathrm{T}}S_{L_2} & \cdots & T_d^{\mathrm{T}}A_1^{\mathrm{T}}S_{L_b} \\ \vdots & \vdots & \ddots & \vdots \\ T_d^{\mathrm{T}}A_b^{\mathrm{T}}S_{L_1} & T_d^{\mathrm{T}}A_b^{\mathrm{T}}S_{L_2} & \cdots & T_d^{\mathrm{T}}A_b^{\mathrm{T}}S_{L_b} \end{pmatrix}.$$

For diagonal block, from Lemma 1,

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

Hence,

$$|(T_d^{\mathrm{T}}A_k^{\mathrm{T}}S_{L_k})_{ij}| \le \frac{q^{2d}-1}{4}\rho_M(T_d). \tag{A.8}$$

For the off-diagonal block, by Lemma 2, for $k \ne l$ and $i,j=1,\ldots,d$,

$$|(T_d^{\mathrm{T}}A_k^{\mathrm{T}}S_{L_l})_{ij}| \le \frac{q^{d-2}(q^2-1)}{4}\left(1+q+\cdots+q^{d-1}\right) = \frac{q^{d-2}(q+1)(q^d-1)}{4}. \tag{A.9}$$

For $\rho_M(T_d) \le q^{d-2}(q+1)/(q^d+1)$, the bound in (A.8) is no more than that in (A.9). For the fourth item of (A.6), it is obvious that for $i,j=1,\ldots,bd$,

$$(S_L^{\mathrm{T}}S_L)_{i,j} \le q^d - 1. \tag{A.10}$$

From (A.7), (A.8), (A.9), and (A.10), we have

$$\rho_M(L_0) \le \frac{\rho_M(T_d)q^d(q^{2d}-1)/12 + q^{d-2}(q+1)(q^d-1)/4 + (q^d-1)/4}{q^d(q^{2d}-1)/12 - (q^{2d}-1)/4 + (q^d-1)/4}$$

$$= \frac{\rho_M(T_d)(q^d+1)}{q^d-2} + \frac{3(q+1)}{q^2(q^d-2)} + \frac{3}{q^d(q^d-2)}.$$

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

$$\begin{aligned} L_1^{\mathrm{T}} L_1 &= ((L+S_L)^{\mathrm{T}}, 1_m, -1_m)((L+S_L)^{\mathrm{T}}, 1_m, -1_m)^{\mathrm{T}} \\ &= L^{\mathrm{T}} L + L^{\mathrm{T}} S_L + S_L^{\mathrm{T}} L + S_L^{\mathrm{T}} S_L + 2 \cdot 1_m 1_m^{\mathrm{T}}, \end{aligned}$$

from (A.7), (A.8), (A.9), and (A.10) we have

$$\begin{aligned} \rho_M(L_1) &\leq \frac{\rho_M(T_d) q^d (q^{2d}-1)/12 + q^{d-2}(q+1)(q^d-1)/2 + (q^d-1) + 2}{q^d(q^{2d}-1)/12 + (q^{2d}-1)/2 + (q^d-1) + 2} \\ &= \frac{\rho_M(T_d) q^d (q^d-1)}{(q^d+2)(q^d+3)} + \frac{6q^{d-2}(q^d-1)(q+1)}{(q^d+1)(q^d+2)(q^d+3)} + \frac{12}{(q^d+2)(q^d+3)}. \end{aligned}$$

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

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