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Construction of orthogonal Latin hypercube designs with flexible run sizes

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ABSTRACT

Latin hypercube designs (LHDs) have recently found wide applications in computer experiments. A number of methods have been proposed to construct LHDs with orthogonality among main-effects. When second-order effects are present, it is desirable that an orthogonal LHD satisfies the property that the sum of elementwise products of any three columns (whether distinct or not) is 0. The orthogonal LHDs constructed by Ye (1998), Cioppa and Lucas (2007), Sun et al. (2009) and Georgiou (2009) all have this property. However, the run size n of any design in the former three references must be a power of two ($n=2^c$) or a power of two plus one ($n=2^c+1$), which is a rather severe restriction. In this paper, we construct orthogonal LHDs with more flexible run sizes which also have the property that the sum of elementwise product of any three columns is 0. Further, we compare the proposed designs with some existing orthogonal LHDs, and prove that any orthogonal LHD with this property, including the proposed orthogonal LHD, is optimal in the sense of having the minimum values of ave($|t|$), $t_{\max}$, ave($|q|$) and $q_{\max}$.

1. Introduction

Latin hypercube designs (LHDs), introduced by McKay et al. (1979), are popular for computer experiments because they allow the investigation of factors at many levels in relatively few trials. An $n\times k$ LHD for k factors in n runs is denoted by an $n\times k$ matrix $L(n, k)=(l_{ij})$, where l_{ij} is the level of factor j in the i th experimental run and each factor in $L(n, k)$ includes n uniformly spaced levels. However, the original construction of LHDs by mating factors randomly is susceptible to having potential high correlations among factors.

Efforts have been made to optimize LHDs. Owen (1992), Tang (1993) and Ma and Zhang (2001) proposed orthogonal array-based LHDs that achieve stratification in low dimensions. Tang (1994) and Morris and Mitchell (1995) proposed LHDs that attain the largest minimum inter-site distance among all LHDs. Park (1994) constructed LHDs that optimize the integrated mean square error criterion. Owen (1994) attempted to lower pairwise correlations between input factors. Tang (1998) considered correlations among higher-order terms derived from the factors. Butler (2001) showed how to construct LHDs in which the terms of a class of trigonometric regression models are orthogonal to one another. Beattie and Lin (1997, 2004, 2005) showed that certain LHDs can be constructed by rotating the points in a two-level full factorial design. Bursztyn and Steinberg (2002) applied the rotation to groups of factors to increase the number of factors in the resulting

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design. Recently, Steinberg and Lin (2006) and Pang et al. (2009) combined the above two ideas with the knowledge of Galois field to produce orthogonal LHDs with n runs, where $n=p^d$, $d=2^c$ and p is a prime. Joseph and Hung (2008) proposed a multi-objective optimization approach to find good LHDs by combining correlation and distance performance measures. Lin et al. (2009) proposed a method for constructing orthogonal or nearly orthogonal LHDs. By relaxing the condition that the number of levels for each factor is identical to the run size, Bingham et al. (2009) introduced a method for constructing a rich class of designs that are suitable for use in computer experiments.

For a polynomial model of degree q, having k factors x_i, $i=1,\ldots,k$,

$$Y=\mu+\sum_{i\le k}\beta_i x_i+\sum_{i_1\le i_2\le k}\beta_{i_1 i_2}x_{i_1}x_{i_2}+\cdots+\sum_{i_1\le\cdots\le i_q\le k}\beta_{i_1\cdots i_q}x_{i_1}\cdots x_{i_q}+\varepsilon,$$

where β_i is the linear effect of x_i, $\beta_{i_1\cdots i_t}$ is the t-order interaction of $x_{i_1},\ldots,x_{i_t}$, in particular β_{ii} corresponds to the quadratic effect of factor x_i and $\beta_{i_1 i_2}$ is the bilinear interaction of factors x_{i_1} and x_{i_2} for $i_1\neq i_2$. It is desirable to include orthogonal independent variables in a regression model, so that the estimates of the regression coefficients would be uncorrelated. When fitting the first-order model, the orthogonal LHD ensures the independence of estimates of linear effects. Furthermore, it is desirable to have an orthogonal LHD that can estimate the linear effects without being correlated with the estimates of quadratic effects and bilinear interactions, when fitting the first-order model while the second-order effects, i.e. the quadratic effects and bilinear interactions, are present. Thus we seek LHDs with the following properties:

(a) the estimates of linear effects of all factors are uncorrelated with each other;
(b) the estimates of linear effects of all factors are uncorrelated with the estimates of all quadratic effects and bilinear interactions.

There are some existing LHDs both with Properties (a) and (b), for example, the $L(2^{c+1}, 2c)$ and $L(2^{c+1}+1, 2c)$ constructed by Ye (1998); the $L(2^{c+1}, 2^c)$ and $L(2^{c+1}+1, 2^c)$ constructed by Sun et al. (2009) for any positive integer c; the $L(2^{c+1},c+1+\binom{c}{2})$ and $L(2^{c+1}+1,c+1+\binom{c}{2})$ for any positive integer $c\le 11$ constructed by Cioppa and Lucas (2007) through extending Ye's procedure; and the LHDs constructed in Georgiou (2009) via (generalized) orthogonal designs. In particular, the number of factors k in any design constructed by Sun et al. (2009) attains its maximum value among all the corresponding LHDs satisfying both Properties (a) and (b).

One limitation of the designs presented in Ye (1998), Cioppa and Lucas (2007) and Sun et al. (2009) is their severe restriction on the run size n, i.e. $n=2^{c+1}$ or $2^{c+1}+1$, which is a rather severe restriction. This paper presents an approach for constructing LHDs with $n=r\,2^{c+1}+1$ or $r\,2^{c+1}$ runs and $k=2^c$ factors for any positive integer r, while still keeping Properties (a) and (b). Note that if an alternative model is employed (e.g., Gaussian process model), the desirable properties may be different and thus the proposed design may not be appropriate.

This paper is organized as follows. Section 2 compares some existing construction methods. In Section 3, we present the construction method of $L(r\,2^{c+1}+1,2^c)$ and $L(r\,2^{c+1}, 2^c)$ with Properties (a) and (b) for any two positive integers c and r. Section 4 provides some criteria for measuring the performance of LHDs, and illustrates that the designs with Properties (a) and (b) perform well under these criteria. Concluding remarks are given in Section 5.

2. Existing methods

We first review the construction method for orthogonal LHDs due to Sun et al. (2009), and then make comparisons with others.

Lemma 1 (*Sun et al., 2009*). (1) *Construction of* $L(2^{c+1}+1, 2^c)$. *For any integer* $c\ge 1$, *the construction algorithm for an orthogonal* $L(2^{c+1}+1, 2^c)$ *with Properties* (a) *and* (b) *can be illustrated as follows.*

Step 1. *For* $c=1$, *let*

$$S_1=\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},\quad T_1=\begin{pmatrix}1 & 2\\ 2 & -1\end{pmatrix}.$$

Step 2. *For* $c>1$, *define* S_c *and* T_c *as*

$$S_c=\begin{pmatrix}S_{c-1} & -S^*_{c-1}\\ S_{c-1} & S^*_{c-1}\end{pmatrix},\quad T_c=\begin{pmatrix}T_{c-1} & -(T^*_{c-1}+2^{c-1}S^*_{c-1})\\ T_{c-1}+2^{c-1}S_{c-1} & T^*_{c-1}\end{pmatrix},$$

where operator * *works on any matrix with an even number of rows by multiplying the entries in the top half of the matrix by* -1 *and leaving those in the bottom half unchanged.*

Step 3. *An* $L(2^{c+1}+1, 2^c)$ *can be obtained as*

$$L_c=(T_c^{\mathrm T},0_{2^c},-T_c^{\mathrm T})^{\mathrm T},$$

where A^{T} denotes the transpose of A and 0_{2^c} denotes the $2^c \times 1$ column vector with all elements zero.

(2) *Construction of $L(2^{c+1}, 2^c)$. For any integer $c \geq 1$, the construction algorithm for an orthogonal $L(2^{c+1}, 2^c)$, L_c, with Properties* (a) *and* (b) *can be illustrated as follows.*

Steps 1′ and 2′. Same as Steps 1 and 2 for construction of S_c and T_c.

Step 3′. Let $H_c = T_c - S_c/2$, $L_c = (H_c^{\mathrm{T}}, -H_c^{\mathrm{T}})^{\mathrm{T}}$.

The number of factors in any of the above constructed designs attains its maximum value among all the corresponding LHDs satisfying both Properties (a) *and* (b).

Suppose $D=(d_{ij})_{n\times k}$ is a fractional factorial design whose levels are taken to be $0,\ldots,p-1$. The corresponding centered design is $D^c=(d_{ij}^c)$, i.e., the levels are labeled as $(2i-p+1)/2$, $i=0,\ldots,p-1$. Let $R=(r_{ij})$ be the corresponding rotation matrix defined in Beattie and Lin (2005) and Pang et al. (2009). Then we have the following conclusion.

Theorem 1. *If D contains three columns d_u, d_v and d_w satisfying $d_u+d_v=d_w \bmod p$, then the resulting design $L=D^cR$ obtained through rotating D^c by R does not satisfy Property* (b).

Proof. Suppose $L=(l_{ij})$ satisfies Property (b). From $D^c=LR'$, for any three columns $d_{j_1}^c$, $d_{j_2}^c$, $d_{j_3}^c$ of D^c, where j_1, j_2, j_3 can be equal, we have

$$\sum_{i=1}^{n} d_{ij_1}^c d_{ij_2}^c d_{ij_3}^c = \sum_{i=1}^{n}\sum_{t_1=1}^{k} l_{it_1} r_{j_1t_1} \sum_{t_2=1}^{k} l_{it_2} r_{j_2t_2} \sum_{t_3=1}^{k} l_{it_3} r_{j_3t_3} = \sum_{t_1=1}^{k}\sum_{t_2=1}^{k}\sum_{t_3=1}^{k} r_{j_1t_1} r_{j_2t_2} r_{j_3t_3} \sum_{i=1}^{n} l_{it_1} l_{it_2} l_{it_3}.$$

From the supposed condition we know that for any three numbers t_1, t_2 and t_3, $\sum_{i=1}^{n} l_{it_1} l_{it_2} l_{it_3} = 0$, where t_1, t_2, t_3 can be equal. Hence,

$$\sum_{i=1}^{n} d_{ij_1}^c d_{ij_2}^c d_{ij_3}^c = 0, \quad \text{for any } j_1, j_2, j_3. \tag{1}$$

On the other hand, let $[x]_p$ denote the residue of x modulo p, then

$$\sum_{i=1}^{n} d_{iu}^c d_{iv}^c d_{iw}^c = \frac{n}{8p^2} \sum_{i=0}^{p-1}\sum_{j=0}^{p-1} (2i-p+1)(2j-p+1)(2[i+j]_p - p+1) = \frac{n}{24}(1-p^2) \neq 0,$$

which contradicts (1), thus we complete the proof. □

From this theorem, we can easily obtain the following result.

Corollary 1. *All the designs $L(p^d, d\lfloor (p^d-1)/d(p-1)\rfloor)$ constructed via the methods of Steinberg and Lin (2006) and Pang et al. (2009) do not satisfy Property* (b) *except for the unique case of $d=p=2$.*

Some comparisons among the LHDs constructed by Ye (1998), Steinberg and Lin (2006), Pang et al. (2009) and Sun et al. (2009) are listed in Tables 1 and 2, where $d=2^c$, c is any positive integer, and p is a prime. In Table 2, several existence results due to Cioppa and Lucas (2007), Lin et al. (2009) and Georgiou (2009) are also listed. For simplicity, we denote the methods of Ye (1998), Cioppa and Lucas (2007), Steinberg and Lin (2006), Pang et al. (2009), Lin et al. (2009), Georgiou (2009) and Sun et al. (2009) by Ye, CL, SL, PLL, LMT, Ge and SLL, respectively. From the above discussions and these two tables, we can see that

(i) in most cases, SLL has a more flexible choice of the number of factors than the other six methods;
(ii) designs due to Ye, CL, Ge and SLL accomplish the nice Properties (a) and (b), and thus they have the minimum values of ave(|t|), $t_{\max}$, ave(|q|) and $q_{\max}$ among all the corresponding LHDs, as will be discussed in Section 4, while those obtained by SL, PLL and LMT only keep Property (a), except the trivial case of $n=4$;
(iii) for $n=2^{c+1}$ or $2^{c+1}+1$ runs, Ye's method can only produce an LHD with at most $k=2c$ factors, while Sun et al. (2009) can generate an LHD with the maximum number of factors among LHDs satisfying both Properties (a) and (b).

Table 1
Comparisons among the construction methods of Ye, SL, PLL and SLL for $n>4$.

Method	Ye	SL	PLL	SLL
Run size n	2^{c+1} or $2^{c+1}+1$	2^d	p^d	2^{c+1} or $2^{c+1}+1$
Maximal number of factors k	$2c$	$d\left\lfloor \frac{n-1}{d} \right\rfloor$	$d\left\lfloor \frac{n-1}{d(p-1)} \right\rfloor$	2^c
Property (a)	Yes	Yes	Yes	Yes
Property (b)	Yes	No	No	Yes
Design optimality[a]	Yes	No	No	Yes

[a] Design optimality means achieving minimum values of ave(|t|), $t_{\max}$, ave(|q|), and $q_{\max}$ simultaneously (see Section 4).

Table 2
Existence of orthogonal LHDs for some given run sizes n.

n	Maximal number of factors k						
	Ye	CL	SL	PLL	LMT	Ge	SLL
8	4					4	4
9	4			4[a]		4	4
16	6	7	12[a]	12[a]		8	8
17	6	7				8	8
32	8	11					16
33	8	11					16
64	10	16			32[a]		32
65	10	16					32
128	12	22					64
129	12	22					64
256	14	29	248[a]	248[a]			128
257	14	29					128
512	16	37					256
513	16	37					256
1024	18	46					512
1025	18	46					512

[a] These designs do not satisfy Property (b), and thus cannot achieve the minimum values of ave($|t|$), $t_{\max}$, ave($|q|$), and $q_{\max}$ simultaneously.

3. Construction of orthogonal LHDs with flexible run sizes

We next extend the method of Sun et al. (2009) presented in Section 2 to construct $L(r\,2^{c+1}, 2^c)$ or $L(r\,2^{c+1}+1, 2^c)$ with Properties (a) and (b), where r and c are two positive integers. This increases the flexibility of the run sizes of the constructed LHDs with Properties (a) and (b).

Suppose T_c is as defined in Lemma 1, and let

$$A_{r2^c\times 2^c} = ((T_c^1)', \ldots, (T_c^r)')',$$

where $T_c^i = T_c + (i-1)2^c S_c$. Then

$$L(r2^{c+1}+1, 2^c) = \begin{pmatrix} A_{r2^c\times 2^c} \\ 0'_{2^c} \\ -A_{r2^c\times 2^c} \end{pmatrix} \tag{2}$$

is an LHD with $r\,2^{c+1}+1$ runs and 2^c factors. From Lemma 1 in Sun et al. (2009), we can easily prove that

Theorem 2. *For any two positive integers c and r, the design given in Eq.* (2) *is an* $L(r\,2^{c+1}+1, 2^c)$ *with Properties* (a) *and* (b).

Example 1 (*Construction of orthogonal L(25,4)*). Since $25 = 3\times 2^{2+1}+1$, from Theorem 2 there exists an LHD with 25 runs and 2^2 factors,

$$L(25,4) = \begin{pmatrix} A_{12\times 4} \\ 0'_4 \\ -A_{12\times 4} \end{pmatrix},$$

with Properties (a) and (b), where

$$A_{12\times 4} = ((T_2^1)', (T_2^2)', (T_2^3)')' = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 2 & -1 & 4 & -3 & 6 & -5 & 8 & -7 & 10 & -9 & 12 & -11 \\ 3 & -4 & -1 & 2 & 7 & -8 & -5 & 6 & 11 & -12 & -9 & 10 \\ 4 & 3 & -2 & -1 & 8 & 7 & -6 & -5 & 12 & 11 & -10 & -9 \end{pmatrix}'.$$

Further, the method can also be modified to construct orthogonal LHDs with $n = r\,2^{c+1}$ runs and $k = 2^c$ factors. Suppose H_c is as defined in Lemma 1, and let

$$B_{r2^c\times 2^c} = ((H_c^1)', \ldots, (H_c^r)')',$$

where $H_c^i = H_c + (i-1)2^c S_c$. Then it can be easily shown that

$$L(r2^{c+1}, 2^c) = \begin{pmatrix} B_{r2^c \times 2^c} \\ -B_{r2^c \times 2^c} \end{pmatrix} \quad (3)$$

is an LHD with $r2_{c+1}$ runs and 2^c factors and has the same nice properties in Theorem 2. Thus, similar to Theorem 2, we conclude that

Theorem 3. *For any two positive integers c and r, the design given in Eq.* (3) *is an* $L(r\,2^{c+1}+1, 2^c)$ *with Properties* (a) *and* (b).

Example 2 (*Construction of orthogonal L(24,4)*). Since $24 = 3 \times 2^{2+1}$, from what we have just discussed, there exists an orthogonal LHD with 24 runs and 2^2 factors,

$$L(24,4) = \begin{pmatrix} B_{12\times 4} \\ -B_{12\times 4} \end{pmatrix},$$

which preserves the nice properties, where

$$B_{12\times 4} = ((H_2^1)', \ (H_2^2)', \ (H_2^3)')'$$
$$= \frac{1}{2}\begin{pmatrix} 1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 & 17 & 19 & 21 & 23 \\ 3 & -1 & 7 & -5 & 11 & -9 & 15 & -13 & 19 & -17 & 23 & -21 \\ 5 & -7 & -1 & 3 & 13 & -15 & -9 & 11 & 21 & -23 & -17 & 19 \\ 7 & 5 & -3 & -1 & 15 & 13 & -11 & -9 & 23 & 21 & -19 & -17 \end{pmatrix}'.$$

Remark. 1. For any $r = 2^l$ with $l > 0$, the $L(2^{c+l+1}+1, 2^{c+l})$ and $L(2^{c+l+1}, 2^{c+l})$ constructed by Sun et al. (2009) have much more choices of factor sizes than the $L(r\,2^{c+1}+1, 2^c)$ and $L(r\,2^{c+1}, 2^c)$ given in Eqs. (2) and (3), respectively. For this case, the designs due to Sun et al. (2009) are recommended.

2. For $r = 2^l m$ with $l > 0$ and m being an odd number, the $L(m\,2^{c+l+1}+1, 2^{c+l})$ and $L(m\,2^{c+l+1}, 2^{c+l})$ instead of the $L(r\,2^{c+1}+1, 2^c)$ and $L(r\,2^{c+1}, 2^c)$ are recommended.

3. (a) If one wants to conduct the experiments from the run size economy point of view, the LHDs with $r=1$ are recommended, in which case the method coincides with that in Sun et al. (2009), see Table 2 for some existence results.

(b) If one prefers to investigate the factors in a more detailed manner (i.e. with more levels) in LHDs, the newly constructed designs with $r > 1$, especially those with odd r, are recommended.

Table 3 shows some existence results of orthogonal LHDs with $n = r\,2^{c+1}$ and $r\,2^{c+1}+1$ for $r=3$, including that obtained by our proposed method. It can be seen that the proposed method has more flexible choices of the run size when compared to other methods.

4. Optimality properties of the constructed LHDs

We now evaluate the performance of the LHDs which are referred to in the previous section. The criteria, as discussed in Steinberg and Lin (2006), arise from the alias matrices when fitting a first-order model while the second-order effects may be present. Let X denote the regression matrix for the first-order model of an $L(n, k)$, including a column of ones and the k factors in the design, which are scaled to the hypercube $[-1,1]^k$. Let X_{int} denote the $n \times k(k-1)/2$ matrix with all the possible bilinear interactions, and let X_{quad} denote the $n \times k$ matrix with all the pure quadratic terms. The alias matrices for the first-order model associated with the bilinear interactions and the pure quadratic terms are then given by

$$T = (X'X)^{-1}X'X_{\text{int}} \quad \text{and} \quad Q = (X'X)^{-1}X'X_{\text{quad}},$$

respectively. A good design for factor screening should maintain relatively small terms in these alias matrices (Steinberg and Lin, 2006). Based on the elements of these matrices, Georgiou (2009) defined the average absolute alias and the maximum absolute alias of the quadratic and the bilinear interactions of a design to evaluate the performance of an LHD. The measures are

$$\text{ave}(|q|) = \frac{\sum_{i=1}^{k+1}\sum_{j=1}^{k}|q_{ij}|}{k(k+1)}, \quad q_{\max} = \max_{i,j}|q_{ij}|$$

Table 3
Existence of orthogonal LHDs with $n=3\cdot 2^{c+1}$ and $3\cdot 2^{c+1}+1$ runs for c=2,…,9.

n	Maximal number of factors k			
	Ye	PLL	LMT	Proposed method
24	4			4
25	4	6[a]	12[a]	4
48	6			8
49	6	8[a]	24[a]	8
96	8			16
97	8			16
192	10			32
193	10			32
384	12			64
385	12			64
768	14			128
769	14			128
1536	16			256
1537	16			256
3072	18			512
3073	18			512

[a] These designs do not satisfy Property (b), and thus cannot achieve the minimum values of ave(|t|), $t_{\max}$, ave(|q|), and $q_{\max}$ simultaneously.

and

$$\text{ave}(|t|)=\frac{2\sum_{i=1}^{k+1}\sum_{j=1}^{k(k-1)/2}|t_{ij}|}{k(k^2-1)},\quad t_{\max}=\max_{i,j}|t_{ij}|,$$

where q_{ij} and t_{ij} are elements in the ith row and jth column of matrices Q and T, respectively. LHDs with smaller values of the above measures of interest are preferred.

For the LHDs with Properties (a) and (b), we can obtain the following result, regarding their quadratic terms and bilinear interactions.

Theorem 4. *If D is an* $L(n,k)$ *possessing Properties* (a) *and* (b), *then D has the minimum values of* ave(|t|), $t_{\max}$, ave(|q|) *and* $q_{\max}$ *among all the orthogonal* $L(n,k)$*'s.*

Proof. For any orthogonal $L(n,k)$, suppose X, X_{int} and X_{quad} are the three matrices previously defined, where the first column of X is the column of ones, and each of the other columns of X is a permutation of $\{-1,-1+2/(n-1),\dots,1-2/(n-1),1\}$. Then the elements in the first row of $X'X_{\text{quad}}$ will all be

$$\alpha=\frac{1}{(n-1)^2}\sum_{i=1}^{n}(2i-n-1)^2=\frac{n(n+1)}{3(n-1)},$$

and the first row of $(X'X)^{-1}$ is $(1/n,0,\dots,0)$. So, the elements in the first row of matrix $Q=(X'X)^{-1}X'X_{\text{quad}}$ will all be α/n for any orthogonal $L(n,k)$. For design D, since it keeps Property (b), all elements of $(X'X)^{-1}X'X_{\text{quad}}$ are 0 except for those in the first row. Thus D has the minimum values of ave(|q|) and $q_{\max}$ among all the orthogonal $L(n,k)$'s.

Since design D satisfies Properties (a) and (b), we have $(X'X)^{-1}X'X_{\text{int}}=0$ and ave(|t|)=$t_{\max}$=0. Thus we complete the proof. □

Theorem 4 tells us that all the LHDs constructed in Section 3 are optimal under the ave(|t|), $t_{\max}$, ave(|q|) and $q_{\max}$ criteria. Further, from this theorem, we can easily verify that if an orthogonal LHD does not satisfy Property (b), then ave(|t|) >0, $t_{\max}>0$, and ave(|q|) cannot take the minimum values. This is true for the orthogonal LHDs constructed via the methods of Steinberg and Lin (2006) and Pang et al. (2009).

5. Concluding remarks

From the newly proposed method, a class of orthogonal $L(n,k)$'s can be constructed algebraically, where $n=r\,2^{c+1}$ or $r\,2^{c+1}+1$, $k=2^c$, and c and r are any two positive integers. Such designs are easy to construct and do not require complicated algorithms to achieve small correlations between input factors. In fact, the estimates of the linear effects of all factors are uncorrelated not only with each other, but also with the estimates of all quadratic effects and bilinear interactions. Further, we prove that the LHDs with Properties (a) and (b) also have the minimum values of ave(|t|), $t_{\max}$, ave(|q|) and $q_{\max}$ among all the orthogonal LHDs with the same run and factor sizes. Such designs can be very useful in factor screening when fitting a first-order model, while the quadratic effects and bilinear interactions exist. In addition, the newly constructed designs enable the experimenters to choose the number of runs with more flexibility.

Joseph and Hung (2008) showed that space-filling property and orthogonality do not necessarily agree with each other, i.e., the uniformity does not guarantee that the design possesses low correlations among its effects; sometimes maximization of inter-site distances can result in LHDs in which the factors are highly correlated, and vice versa. The proposed designs can only guarantee the nice orthogonality properties, and thus are optimal in terms of all design criteria based on orthogonality.

For the analysis of the computer experiments, one could focus on the mean model (such as what we have concerned here) and assume a relative simple form for the covariance structure. In this case, a polynomial model is commonly employed. The proposed design is shown to be effective. On the hand, one could assume a simple mean model (e.g., an intercept only) with a relative complicated covariance structure, such as a Gaussian process model. In this case, whether the proposed orthogonal LHD will be beneficial deserves further study.

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