

A New and Flexible Method for Constructing Designs for Computer Experiments

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Abstract

We develop a new method for constructing “good” designs for computer experiments. The method derives its power from its basic structure that builds large designs using small designs. We specialize the method for the construction of orthogonal Latin hypercubes and obtain many results along the way. In terms of run sizes, the existence problem of orthogonal Latin hypercubes is completely solved. We also present an explicit result showing how large orthogonal Latin hypercubes can be constructed using small orthogonal Latin hypercubes. Another appealing feature of our method is that it can easily be adapted to construct other designs; we examine how to make use of the method to construct nearly orthogonal and cascading Latin hypercubes.

Key words and phrases: Cascading Latin hypercube; Hadamard matrix; Kronecker product; Orthogonal array; Orthogonal Latin hypercube; Space-filling design.

1. Introduction

Scientists are increasingly using experiments on computer simulators to help understand physical systems. Computer experiments differ from physical experiments in that the systems are usually deterministic, and thus the response in computer experiments is unchanged if a design point is replicated. The lack of random error presents challenges to both the design and analysis of experiments (e.g., see Sacks et al., 1989).

Similar to physical experiments, computer experiments are performed with a variety of goals in mind. Objectives include factor screening (Welch et al., 1992; Linkletter et al., 2006), building an emulator of the simulator (Sacks et al., 1989), optimization (Jones, Schonlau and Welch, 1998), and model calibration (Kennedy and O’Hagan, 2001). Latin hypercube designs

(McKay, Beckman and Conover, 1979) are commonly used for computer experiments. These designs have the feature that when projected onto one dimension, the equally spaced design points ensure that each of the input variables has all portions of its range represented.

While constructing Latin hypercube designs is fairly easy, it is more challenging to find these designs when optimality criteria are imposed. Ye (1998), Steinberg and Lin (2006) and Cioppa and Lucas (2007) developed methods for constructing orthogonal Latin hypercubes. These methods all have restrictions on the run size n . The approach of Ye (1998) and Cioppa and Lucas (2007) gives designs for $n = 2^k$ or $2^k + 1$ and the method of Steinberg and Lin (2006) provides designs for $n = 2^{2^k}$, where $k \geq 2$ is an integer. Practitioners would appreciate a methodology that can quickly produce designs with more flexible run sizes.

In this article, a new construction is proposed for finding “good” Latin hypercube designs for computer experiments. The method is simple and uses small designs to construct larger designs with desirable properties. Our methodology is quite powerful insofar as it allows orthogonal Latin hypercubes to be constructed for any run size n where $n \neq 4k + 2$. When $n = 4k + 2$, we prove that an orthogonal Latin hypercube does not exist. Another important feature of our method is that it can easily be adapted to construct nearly orthogonal Latin hypercubes and cascading Latin hypercubes (Handcock, 1991).

The article is outlined as follows. Section 2 introduces notation, presents a general method of construction and discusses how to obtain Latin hypercubes based on this general structure. Section 3 devotes itself to the construction of orthogonal Latin hypercubes. Besides several general theoretical results and many concrete examples, an existence result is also established here. In Section 4, we examine how the general method can be used to construct nearly orthogonal and cascading Latin hypercubes. We conclude the article with some remarks in Section 5. The proofs for some theoretical results are deferred to Appendix A for a smooth flow of the main ideas and results.

2. A General Method of Construction

Consider designs of n runs with m factors of s levels, where $2 \leq s \leq n$. Without loss of generality, the s levels are taken to be centered at zero and equally-spaced. For odd

s , the levels are taken as $-(s-1)/2, \dots, -1, 0, 1, \dots, (s-1)/2$ and for even s , they are $-(s-1)/2, \dots, -1/2, 1/2, \dots, (s-1)/2$. The levels except for level 0 in the case of odd s are assumed to be equally replicated in each design column to ensure that linear main effects are all orthogonal to the grand mean. Such a design is denoted by $D(n, s^m)$ and can be represented by an $n \times m$ matrix $D = (d_{ij})$ with entries from the set of s levels as described above. In this notation, an m -factor Latin hypercube design is a $D(n, s^m)$ with $n = s$.

2.1 Construction method

Let $A = (a_{ij})_{n_1 \times m_1}$ be a matrix with entries $a_{ij} = \pm 1$, $B = (b_{ij})_{n_2 \times m_2}$ be a $D(n_2, s_2^{m_2})$, $C = (c_{ij})_{n_1 \times m_1}$ be a $D(n_1, s_1^{m_1})$, and $D = (d_{ij})_{n_2 \times m_2}$ be a matrix with entries $d_{ij} = \pm 1$. Let γ be a real number. New designs are found using the following construction:

$$L = A \otimes B + \gamma C \otimes D, \quad (1)$$

where Kronecker product $A \otimes B$ is the $n_1 n_2 \times m_1 m_2$ matrix

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1m_1}B \\ a_{21}B & a_{22}B & \dots & a_{2m_1}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{n_1 1}B & a_{n_1 2}B & \dots & a_{n_1 m_1}B \end{bmatrix}$$

with $a_{ij}B$ itself being an $n_2 \times m_2$ matrix. The resulting design L in (1) has $n = n_1 n_2$ runs and $m = m_1 m_2$ factors.

The above construction has an interesting interpretation. As an illustration, consider a simple case in which $A = (1, 1)^T$ and $C = (1/2, -1/2)^T$. Design L in (1) has a column

$$\begin{pmatrix} b + \frac{\gamma}{2}d \\ b - \frac{\gamma}{2}d \end{pmatrix}, \quad (2)$$

where b is a column of B and d is a column of D . Further let $d = (d_1, \dots, d_{n_2})^T$. Since $d_i = \pm 1$, the column (2) can be viewed as simultaneously shifting each level in b to the left and the right by $\gamma/2$. If we view b as a block of level settings, then we are shifting two identical blocks b , one to the left and the other to the right. We will show in Section 2.2 that with the appropriate

choices of A , B , C , D and γ , the levels in each column of L in (1) are equally-spaced and unreplicated, thus resulting in a Latin hypercube.

Now consider all m columns of L under this simple case. Each one-dimensional block b becomes an m -dimensional stratum, B . Suppose D is a matrix of plus ones. Then the design points in $B + \gamma D/2$ can be obtained by shifting the entire stratum B to the right by $\gamma/2$. Similarly, the design points in $B - \gamma D/2$ can be obtained by shifting the entire stratum B to the left by $\gamma/2$. In this case, closely clustered points in each stratum are expected. This feature can be utilized to construct cascading Latin hypercubes (Lin 2008).

We shall see that the orthogonality or near orthogonality of L in (1) is determined by the orthogonality or near orthogonality of A , B , C and D , the correlations between the columns in A and those in C , and the correlations between the columns in B and those in D . As a result, the method allows orthogonal and nearly orthogonal Latin hypercubes to be easily constructed.

Vartak (1955) appears to be the first to use Kronecker product systematically to construct statistical experimental designs. In a recent work, Bingham, Sitter and Tang (2009) introduced a method for constructing a rich class of designs that are suitable for use in computer experiments. Their approach corresponds to $\gamma = 0$ in the general construction given in (1). The designs in that paper have many levels and are not Latin hypercubes in general.

2.2 Latin hypercubes

The following result shows how to obtain Latin hypercubes from the construction in (1).

Lemma 1. *Let $\gamma = n_2$. Then design L in (1) is a Latin hypercube if*

(i) *both B and C are Latin hypercubes and*

(ii) *at least one of the following two conditions is true:*

(a) *A and C satisfy that for any i , if p and p' are such that $c_{pi} = -c_{p'i}$, then $a_{pi} = a_{p'i}$;*

(b) *B and D satisfy that for any j , if q and q' are such that $b_{qj} = -b_{q'j}$, then $d_{qj} = d_{q'j}$.*

The proof is given in Appendix A. Just in terms of constructing Latin hypercubes, Lemma 1 is not of much significance in itself as one can easily obtain a Latin hypercube simply by combining several permutations of the set of levels. The significance of Lemma 1 lies in the fact that it produces Latin hypercubes with the structure in (1) and thus provides a path to

the construction of orthogonal and cascading Latin hypercubes.

Condition (i) in Lemma 1 is not really a condition, and it simply tells us to choose B and C to be Latin hypercubes. In order for L to be a Latin hypercube, the only mild condition is that in (ii) of Lemma 1. Two situations where condition (ii) is obviously met are as follows: (α) C has a foldover structure in the sense that $C = (C_0^T, -C_0^T)^T$ and A has form $A = (A_0^T, A_0^T)^T$; (β) A or D is a matrix of all plus ones. Both situations are useful. Theorem 3 of Section 3.3 is derived under situation (α). Situation (β) can be used for constructing cascading Latin hypercubes. We now give an example to illustrate Lemma 1.

Example 1. Consider the construction of Latin hypercubes of 32 runs with 32 factors. We choose $n_1 = m_1 = 2$ and $n_2 = m_2 = 16$ so that $n = n_1 n_2 = 32$ and $m = m_1 m_2 = 32$. To meet condition (ii) in Lemma 1, let A be a matrix of all plus ones. Now let $\gamma = n_2 = 16$ and $D = (d_{ij})$ be any 16×16 matrix of ± 1 . For L in (1) to be a Latin hypercube, we need both B and C to be Latin hypercubes. Let us use $C = [(1/2, -1/2)^T, (-1/2, 1/2)^T]^T$ and

$$B = \frac{1}{2} \begin{pmatrix} -15 & 5 & 9 & -3 & 7 & 11 & -11 & 7 & -9 & 3 & -15 & 5 & 11 & -11 & 7 & -7 \\ -13 & 1 & 1 & 13 & -7 & -11 & 11 & -7 & -1 & -13 & -13 & 1 & 13 & 5 & 5 & -3 \\ -11 & 7 & -7 & -11 & 13 & -1 & -1 & -13 & 9 & -3 & 15 & -5 & -5 & 11 & -7 & 7 \\ -9 & 3 & -15 & 5 & -13 & 1 & 1 & 13 & 1 & 13 & 13 & -1 & -13 & -5 & -5 & 3 \\ -7 & -11 & 11 & -7 & 11 & -7 & 7 & 11 & 5 & 15 & -3 & -9 & -9 & 3 & 9 & 11 \\ -5 & -15 & 3 & 9 & -11 & 7 & -7 & -11 & 13 & -1 & -1 & -13 & -1 & 9 & 11 & 15 \\ -3 & -9 & -5 & -15 & 1 & 13 & 13 & -1 & -5 & -15 & 3 & 9 & 1 & 7 & -11 & -11 \\ -1 & -13 & -13 & 1 & -1 & -13 & -13 & 1 & -13 & 1 & 1 & 13 & 9 & -9 & -9 & -15 \\ 1 & 13 & 13 & -1 & -9 & 3 & -15 & 5 & 11 & -7 & 7 & 11 & -7 & -7 & -15 & -9 \\ 3 & 9 & 5 & 15 & 9 & -3 & 15 & -5 & 3 & 9 & 5 & 15 & -15 & -13 & -13 & -13 \\ 5 & 15 & -3 & -9 & -3 & -9 & -5 & -15 & -11 & 7 & -7 & -11 & 15 & -3 & 15 & 9 \\ 7 & 11 & -11 & 7 & 3 & 9 & 5 & 15 & -3 & -9 & -5 & -15 & 7 & 15 & 13 & 13 \\ 9 & -3 & 15 & -5 & -5 & -15 & 3 & 9 & -7 & -11 & 11 & -7 & 5 & 13 & -3 & 5 \\ 11 & -7 & 7 & 11 & 5 & 15 & -3 & -9 & -15 & 5 & 9 & -3 & 3 & -1 & -1 & 1 \\ 13 & -1 & -1 & -13 & -15 & 5 & 9 & -3 & 7 & 11 & -11 & 7 & -11 & -15 & 3 & -5 \\ 15 & -5 & -9 & 3 & 15 & -5 & -9 & 3 & 15 & -5 & -9 & 3 & -3 & 1 & 1 & -1 \end{pmatrix}. \quad (3)$$

According to Lemma 1, design L in (1) is then a 32×32 Latin hypercube.

3. Constructing Orthogonal Latin hypercubes

We first consider in Section 3.1 the construction of orthogonal Latin hypercubes with run sizes n that are multiples of eight. The results here are offered directly by the construction in (1). In Section 3.2, additional techniques are employed for constructing orthogonal Latin hypercubes of other run sizes. Results from the application of the methods in Sections 3.1 and 3.2 are presented in Section 3.3.

3.1 Orthogonal Latin hypercubes of $n = 8k$ runs

A design or matrix $X = (x_1, \dots, x_m)$ is said to be orthogonal if the inner product of any two columns is zero, that is, $x_i^T x_j = 0$ for all $i \neq j$. The next result provides a set of sufficient conditions for design L in (1) to be orthogonal.

Lemma 2. *Design L in (1) is orthogonal if*

- (i) A, B, C and D are all orthogonal, and
- (ii) at least one of the two, $A^T C = 0$ and $B^T D = 0$, holds.

The proof is simple, making use of the following properties of Kronecker product:

$$(A \otimes B)^T = A^T \otimes B^T; \quad \text{and} \quad (A \otimes B)(C \otimes D) = (AC) \otimes (BD). \quad (4)$$

Lemma 1 tells how to make L in (1) a Latin hypercube whereas Lemma 2 tells how to make it orthogonal. When the two lemmas are combined, we have a way of obtaining orthogonal Latin hypercubes.

Theorem 1. *Let $\gamma = n_2$. Then design L in (1) is an orthogonal Latin hypercube if*

- (i) A and D are orthogonal matrices of ± 1 ,
- (ii) B and C are orthogonal Latin hypercubes,
- (iii) at least one of the two, $A^T C = 0$ and $B^T D = 0$, is true, and
- (iv) at least one of the following two conditions is true:
 - (a) A and C satisfy that for any i , if p and p' are such that $c_{pi} = -c_{p'i}$, then $a_{pi} = a_{p'i}$;
 - (b) B and D satisfy that for any j , if q and q' are such that $b_{qj} = -b_{q'j}$, then $d_{qj} = d_{q'j}$.

The role played by A and D is very different from that of B and C in Theorem 1. To help understand Theorem 1, one may think that B and C are the building material while A and D provide a blueprint for the construction. Small orthogonal Latin hypercubes B and C are used to construct a large orthogonal Latin hypercube L in Theorem 1. Exactly how the construction is accomplished is guided by A and D , which are orthogonal matrices of ± 1 . In addition to the right blueprint and building material, considerable amount of care is necessary for the final structure to be right. This is achieved via $\gamma = n_2$ and conditions (iii) and (iv) in Theorem 1.

Note that A and D may or may not be square matrices and the orthogonality of A and D is imposed on their columns. In some mathematics literature, such matrices are called Hadamard submatrices. For convenience, we simply call A or D an orthogonal matrix when its columns are orthogonal. Hadamard matrices and orthogonal arrays with levels ± 1 are all such orthogonal matrices in our terminology. A Hadamard matrix is a square orthogonal matrix of ± 1 . An orthogonal array with two levels ± 1 requires that each of the four combinations $(-1, -1)$, $(-1, +1)$, $(+1, -1)$ and $(+1, +1)$ occurs the same number of times in every two columns. For some comprehensive discussion on these and other topics in the theory of factorial designs, we refer to Dey and Mukerjee (1999), Hedayat, Sloane and Stufken (1999) and Mukerjee and Wu (2006).

Because of the orthogonality of A and D , we must have that n_1 and n_2 are equal to two or multiples of four. The case where $n_1 = n_2 = 2$ is trivial. Consequently, Theorem 1 can be used to construct orthogonal Latin hypercubes of $n = 8k$ runs, thereby providing designs that are unavailable in Ye (1998) and Steinberg and Lin (2006). When $n = n_1 n_2$ is a multiple of 16, Theorem 1 becomes more powerful. This point will be highlighted in Section 3.3. We now revisit Example 1 for an illustration of Theorem 1.

Example 2. In Example 1, the first 12 columns of B form a 16-run orthogonal Latin hypercube constructed by Steinberg and Lin (2006). If D is chosen to be a Hadamard matrix of order 16 in Example 1, Theorem 1 tells us the first 12 columns of L in Example 1 constitute a 32×12 orthogonal Latin hypercube, which has one more orthogonal factor than the 32×11 orthogonal Latin hypercube obtained by Cioppa and Lucas (2007).

When $n_1 = n_2$, a stronger result than Theorem 1 can be established, again using the properties of Kronecker product given in (4).

Proposition 1. *If $n_1 = n_2 = n_0$ and A, B, C, D and γ are chosen according to Theorem 1, then design (L, U) is an orthogonal Latin hypercube with $2m_1 m_2$ factors, where L is as in Theorem 1 and $U = -n_0 A \otimes B + C \otimes D$.*

We now discuss how to choose A, B, C, D and γ to construct orthogonal Latin hypercubes. According Theorem 1, we have that $\gamma = n_2$. Matrices A and D need to be orthogonal with

entries of ± 1 . As discussed earlier, two level orthogonal arrays and Hadamard matrices are all such orthogonal matrices. Theorem 1 requires that designs B and C be orthogonal Latin hypercubes. All known orthogonal Latin hypercubes from the existing literature can be used here. Later in this paper (see Table 2), we obtain a collection of small orthogonal Latin hypercubes through computer search for this purpose. So far, all are straightforward. The nontrivial aspect from applying Theorem 1 is to satisfy conditions (iii) and (iv) which require that A and C (or B and D) jointly have certain properties. In this paper, we satisfy these two conditions by choosing A of form $A = (A_0^T, A_0^T)^T$ and C of form $C = (C_0^T, -C_0^T)^T$ where A_0 and C_0 are such that all the columns in the matrix

$$(A, C) = \begin{bmatrix} A_0 & C_0 \\ A_0 & -C_0 \end{bmatrix} \quad (5)$$

are mutually orthogonal. In Section 3.3 we provide a method of finding such orthogonal matrices with the structure in (5) when proving Theorem 3. Comments similar to those in this paragraph can also be made regarding the application of Proposition 2 in Section 3.2.

3.2 Orthogonal Latin hypercubes with other run sizes

Consider an orthogonal Latin hypercube of n runs with $m \geq 2$ factors. Trivially, run size n cannot be two or three. So we must have $n \geq 4$. The next result provides a complete characterization of the existence of an orthogonal Latin hypercube in terms of run size n .

Theorem 2. *There exists an orthogonal Latin hypercube of $n \geq 4$ runs with more than one factor if and only if $n \neq 4k + 2$ for any integer k .*

Appendix A contains a proof for Theorem 2. Equivalently, Theorem 2 says that the run size of an orthogonal Latin hypercube has to be odd or a multiple of 4. Theorem 1 provides a method for constructing orthogonal Latin hypercubes of $n = 8k$ runs. The present section examines how to construct orthogonal Latin hypercubes of other run sizes.

The basic idea of our method is quite simple. To obtain an orthogonal Latin hypercube, we stack up two orthogonal designs with mutually exclusive and exhaustive sets of levels. To make it precise, we use \mathcal{S} to denote the set of n levels of a Latin hypercube of n runs. Let

$\mathcal{S} = \mathcal{S}_a \cup \mathcal{S}_b$ where $\mathcal{S}_a \cap \mathcal{S}_b = \phi$, and let n_a and n_b be the numbers of levels in \mathcal{S}_a and \mathcal{S}_b , respectively. Suppose that there exist an $n_a \times m$ orthogonal design D_a with levels in \mathcal{S}_a and an $n_b \times m$ orthogonal design D_b with levels in \mathcal{S}_b , where for both D_a and D_b , each level appears precisely once within each column. Then

$$L = \begin{pmatrix} D_a \\ D_b \end{pmatrix} \quad (6)$$

is an $n \times m$ orthogonal Latin hypercube with $n = n_a + n_b$. Note that D_a and D_b themselves are not necessarily Latin hypercubes.

We consider two special choices for \mathcal{S}_a and \mathcal{S}_b . For easy reference later in the paper, we call them two stacking methods. Our first stacking method chooses n_a and n_b such that $|n_a - n_b| = 1$, with the corresponding $\mathcal{S}_a = \{-(n_a - 1), -(n_a - 3), \dots, n_a - 3, n_a - 1\}$ and $\mathcal{S}_b = \{-(n_b - 1), -(n_b - 3), \dots, n_b - 3, n_b - 1\}$. This implies that both $D_a/2$ and $D_b/2$ in (6) are orthogonal Latin hypercubes. We may assume that n_a is odd and n_b is even in the above. By Theorem 2, we know that n_b has form $4k$. It follows that n_a has form $4k - 1$ or $4k + 1$. Thus, the first stacking method allows orthogonal Latin hypercubes of run sizes $8k - 1$ and $8k + 1$ to be constructed.

The second stacking method is more generally applicable and it chooses $\mathcal{S}_a = \{-(n_a - 1)/2, -(n_a - 3)/2, \dots, (n_a - 3)/2, (n_a - 1)/2\}$ and

$$\mathcal{S}_b = \{-(n_a + n_b - 1)/2, \dots, -(n_a + 1)/2, (n_a + 1)/2, \dots, (n_a + n_b - 1)/2\}. \quad (7)$$

For this choice, D_a is an orthogonal Latin hypercube while D_b is not. We examine how to construct an orthogonal design D_b with level set \mathcal{S}_b given in (7). Now consider the matrices in Table 1. Each of the four matrices in Table 1 has the following properties: (i) it has real entries $\pm x_1, \dots, \pm x_{n/2}$, (ii) both x_i and $-x_i$ occur exactly once in each column and (iii) every two columns are orthogonal. We note that the matrices in Table 1 are related to but different from orthogonal designs in the combinatorics literature (Geramita and Seberry, 1979).

The matrices in Table 1 can be used to construct orthogonal Latin hypercubes of n runs by setting $x_i = (2i - 1)/2$ for $i = 1, \dots, n/2$. They also provide a direct construction of orthogonal designs D_b with level set \mathcal{S}_b in (7) by choosing $x_i = (n_a + 2i - 1)/2$ for $i = 1, \dots, n_b/2$. Most

Table 1. Four useful matrices

n														
2	4		8				16							
x_1	x_1	x_2	x_1	$-x_2$	x_4	x_3	x_1	$-x_2$	$-x_4$	$-x_3$	$-x_8$	x_7	x_5	x_6
$-x_1$	x_2	$-x_1$	x_2	x_1	x_3	$-x_4$	x_2	x_1	$-x_3$	x_4	$-x_7$	$-x_8$	$-x_6$	x_5
	$-x_1$	$-x_2$	x_3	$-x_4$	$-x_2$	$-x_1$	x_3	$-x_4$	x_2	x_1	$-x_6$	$-x_5$	x_7	$-x_8$
	$-x_2$	x_1	x_4	x_3	$-x_1$	x_2	x_4	x_3	x_1	$-x_2$	$-x_5$	x_6	$-x_8$	$-x_7$
			$-x_1$	x_2	$-x_4$	$-x_3$	x_5	$-x_6$	$-x_8$	x_7	x_4	x_3	$-x_1$	$-x_2$
			$-x_2$	$-x_1$	$-x_3$	x_4	x_6	x_5	$-x_7$	$-x_8$	x_3	$-x_4$	x_2	$-x_1$
			$-x_3$	x_4	x_2	x_1	x_7	$-x_8$	x_6	$-x_5$	x_2	$-x_1$	$-x_3$	x_4
			$-x_4$	$-x_3$	x_1	$-x_2$	x_8	x_7	x_5	x_6	x_1	x_2	x_4	x_3
							$-x_1$	x_2	x_4	x_3	x_8	$-x_7$	$-x_5$	$-x_6$
							$-x_2$	$-x_1$	x_3	$-x_4$	x_7	x_8	x_6	$-x_5$
							$-x_3$	x_4	$-x_2$	$-x_1$	x_6	x_5	$-x_7$	x_8
							$-x_4$	$-x_3$	$-x_1$	x_2	x_5	$-x_6$	x_8	x_7
							$-x_5$	x_6	x_8	$-x_7$	$-x_4$	$-x_3$	x_1	x_2
							$-x_6$	$-x_5$	x_7	x_8	$-x_3$	x_4	$-x_2$	x_1
							$-x_7$	x_8	$-x_6$	x_5	$-x_2$	x_1	x_3	$-x_4$
							$-x_8$	$-x_7$	$-x_5$	$-x_6$	$-x_1$	$-x_2$	$-x_4$	$-x_3$

importantly, they are useful in the following result that allows us to construct D_b with level set \mathcal{S}_b in (7) for more general n_b .

Proposition 2. *Let $\gamma = 1$. Then design L in (1) is an orthogonal design with level set $\{-(n_a + n - 1)/2, \dots, -(n_a + 1)/2, (n_a + 1)/2, \dots, (n_a + n - 1)/2\}$ if*

- (i) *A and D are orthogonal matrices of ± 1 ,*
- (ii) *B is an orthogonal Latin hypercube and C is an orthogonal design with level set $\pm(n_a + n_2)/2, \pm(n_a + 3n_2)/2, \dots, \pm(n_a + (n_1 - 1)n_2)/2$,*
- (iii) *at least one of the two, $A^T C = 0$ and $B^T D = 0$, is true, and*
- (iv) *at least one of the following two conditions is true:*

- (a) *A and C satisfy that for any i , if p and p' are such that $c_{pi} = -c_{p'i}$, then $a_{pi} = a_{p'i}$;*
- (b) *B and D satisfy that for any j , if q and q' are such that $b_{qj} = -b_{q'j}$, then $d_{qj} = d_{q'j}$.*

Orthogonality of design L follows from Lemma 2. That L has a desired set of levels can easily be established, which follows a similar path to that for Lemma 1. Comparing Proposition 2 with Theorem 1, we see that the only changes are those made to γ and C . Mathematically, Theorem 1 is a special case of Proposition 2 as one can obtain the former from the latter by

setting $n_a = 0$. We present them separately because they carry different messages and serve different purposes in this paper.

Design C required in Proposition 2 can easily be obtained from the matrices in Table 1. By letting $n = n_b$ in Proposition 2, design L in Proposition 2 can then be used as our D_b as it has desired level set \mathcal{S}_b in (7). The run size n_b of such D_b has form $n_b = 8k$. Since there is no restriction in the run size n_a of D_a other than that D_a is an orthogonal Latin hypercube, this second stacking method allows orthogonal Latin hypercubes of any run size $n \neq 4k + 2$ to be constructed.

Example 3. In Example 2, if we choose $\gamma = 1$ and let $C = (-17/2, 17/2)^T$, Proposition 2 gives an orthogonal design D_b of $n_b = 32$ runs for 12 factors, where each column of D_b is a permutation of $-16, -15, \dots, -1, 1, \dots, 15, 16$. Now let $n_a = 1$ and D_a be a row of zeros. Then stacking up D_a and D_b gives a 33×12 orthogonal Latin hypercube.

3.3 Some results

The methods in Sections 3.1 and 3.2 both build large orthogonal Latin hypercubes from small ones. To apply the methods, we need to find orthogonal Latin hypercubes with small runs. Various efficient algorithms can be helpful in this regard. Lin (2008) reported an algorithm adapted from that of Xu (2002). The key idea of the algorithm is to add columns sequentially to an existing design. To add a column, two operations, pairwise switch and exchange, are used. A pairwise switch switches a pair of distinct levels in a column. For a candidate column, the algorithm searches for all possible pairwise switches and makes the pairwise switch that achieves the best improvement. This search and pairwise switch procedure is repeated until an orthogonal Latin hypercube is found. An exchange replaces the candidate column by a randomly generated column. The exchange step is repeated at most T_1 (user-specified) times if no orthogonal Latin hypercube is obtained. Since the procedure relies on the initial random columns, the entire procedure is repeated T_2 times. Apart from the sequential idea, the efficiency of the algorithm benefits from its fast updates of orthogonality. An update is needed when a pairwise switch is applied. The maximum number m of the columns in orthogonal Latin hypercubes of n runs found by the algorithm is given in Table 2 for $4 \leq n \leq 21$ except for $n = 16$, in which case, our algorithm finds $m = 6$. The entry $m = 12$ for $n = 16$ in Table 2 is due

to Steinberg and Lin (2006). The detailed design matrices for the orthogonal Latin hypercubes in Table 2 are presented in Lin (2008) and also available from the authors.

Table 2. The maximum number m of columns in $OLH(n, m)$ by the algorithm for $4 \leq n \leq 21$

n	4	5	7	8	9	11	12	13	15	16	17	19	20	21
m	2	2	3	4	5	7	6	6	6	12	6	6	6	6

For a concise presentation of the results in this section, we use $OLH(n, m)$ to denote an orthogonal Latin hypercube of n runs for m factors. We now present a general result from the application of Theorem 1 in Section 3.1 and the second stacking method in Section 3.2.

Theorem 3. *Suppose that an $OLH(n, m)$ is available, where n is a multiple of 4 such that a Hadamard matrix of order n exists. Then we have that*

- (i) *the following orthogonal Latin hypercubes, an $OLH(2n, m)$, an $OLH(4n, 2m)$, an $OLH(8n, 4m)$ and an $OLH(16n, 8m)$, can all be constructed;*
- (ii) *all the following orthogonal Latin hypercubes, an $OLH(2n + 1, m)$, an $OLH(4n + 1, 2m)$, an $OLH(8n + 1, 4m)$ and an $OLH(16n + 1, 8m)$ can also be constructed.*

We give a proof for Theorem 3. The proof in fact provides a detailed procedure for the actual construction of these orthogonal Latin hypercubes. Part (i) of Theorem 3 results from an application of Theorem 1 in Section 3.1. In the general construction (1), we choose B to be the given $OLH(n, m)$. Matrix D is obtained by taking m columns from a Hadamard matrix of order n . Design C is chosen to be an orthogonal Latin hypercube derived from a matrix in Table 1. Note that each of the four matrices in Table 1 has a fold-over structure in that it can be written as $(X^T, -X^T)^T$. Now let $A = (S^T, S^T)^T$, where S is obtained from X by setting $x_i = 1$ for all i . With the above choices for A , B , C and D , conditions (i), (ii), (iii) and (iv) in Theorem 1 are all satisfied. This proves part (i) of Theorem 3. The proof for part (ii) of Theorem 3 is similar, involving the second stacking method with $n_a = 1$ and an application of Proposition 2.

Theorem 3 is a very powerful result. By repeated application of Theorem 3, one can obtain many infinite series of orthogonal Latin hypercubes. For example, starting with an $OLH(12, 6)$

from Table 2, we can obtain an OLH(192, 48), which can be used in turn to construct an OLH(768, 96) and so on. For another example, an OLH(256, 248) in Steinberg and Lin (2006) can be used to construct an OLH(1024, 496), an OLH(4096, 1984) and so on.

One important problem in the study of orthogonal Latin hypercubes is to determine the maximum number m^* of factors for an OLH(n, m^*) to exist. Theorem 2 says that $m^* = 1$ if n is 3 or has form $n = 4k + 2$ and that $m^* \geq 2$ otherwise. This result is now strengthened below.

Proposition 3. *The maximum number m^* of factors for an orthogonal Latin hypercube of $n = 16k + j$ runs has a lower bound given below:*

- (i) $m^* \geq 6$ for all $n = 16k + j$ where $k \geq 1$ and $j \neq 2, 6, 10, 14$;
- (ii) $m^* \geq 7$ for $n = 16k + 11$ where $k \geq 0$;
- (iii) $m^* \geq 12$ for $n = 16k, 16k + 1$ where $k \geq 2$;
- (iv) $m^* \geq 24$ for $n = 32k, 32k + 1$ where $k \geq 2$;
- (v) $m^* \geq 48$ for $n = 64k, 64k + 1$ where $k \geq 2$.

Part (i) of Proposition 3 is obtained as follows. By our second stacking method with the use of the 16×8 matrix in Table 1, we can construct an OLH($n + 16, m$) where $m \leq 8$ if an OLH(n, m) is available. Part (i) of Proposition 3 will be true if we can claim that an OLH($n, 6$) exists for all $17 \leq n \leq 32$ except for $n = 18, 22, 26, 30$. We already know that the claim is true for $n = 17, 19, 20, 21$ from Table 2 and for $n = 32$ from Example 2. Note that an OLH(11, 6) can be obtained by choosing any six columns from the OLH(11, 7) in Table 2. For $n = 23$, we use the first stacking method by choosing $n_a = 11$ and $n_b = 12$ and using an OLH(11, 6) and the OLH(12, 6) in Table 2. The case $n = 24$ follows from applying part (i) of Theorem 3 to the OLH(12, 6) in Table 2. For $n = 25$, an OLH(25, 6) can be constructed using the first stacking method with $n_a = 13$ and $n_b = 12$. For $n = 27$, we apply the second stacking method by choosing $n_a = 11$ and $n_b = 16$. The second stacking method also allows the construction of an OLH(28, 6), an OLH(29, 6) and an OLH(31, 6). We choose $n_a = 12$ and $n_b = 16$ for $n = 28$, $n_a = 13$ and $n_b = 16$ for $n = 29$, and $n_a = 15$ and $n_b = 16$ for $n = 31$. Part (ii) follows from the existence of an OLH(11, 7) in Table 2. Parts (iii), (iv) and (v) follows from an application of Theorem 3.

Table 3. Orthogonal Latin hypercubes of $n = 16k$ runs where $k \geq 2$

n	m	Ye	SL	CL
32	12	8	0	9
48	12	0	0	0
64	32*	10	0	16
80	12	0	0	0
96	24	0	0	0
112	12	0	0	0
128	48	12	0	22
144	24*	0	0	0
160	24	0	0	0
176	12	0	0	0
192	48	0	0	0
208	12	0	0	0
224	24	0	0	0
240	12	0	0	0
256	192*	14	248	29

Note: Ye: the number of orthogonal columns by Ye (1998)

SL: the number of orthogonal columns by Steinberg and Lin (2006)

CL: the number of orthogonal columns by Cioppa and Lucas (2007)

The following remarks are in order regarding Proposition 3. If we wish, we can obtain sharper lower bounds on m^* for certain values of n by applying Theorem 3. For example, using the OLH(12,6) in Table 2, we can establish that $m^* \geq 6 \times 8^k$ for $n = 12 \times 16^k$. We will not dwell further on this issue but are satisfied with the general lower bound in Proposition 3. The lower bound in Proposition 3 is derived from the small orthogonal Latin hypercubes found by our algorithm. Therefore, improved bounds will be naturally available in the future if better results are obtained from computer search.

Lin (2008) in her thesis provides a comprehensive table of orthogonal Latin hypercubes for all $n \leq 256$. Here we present the results in Table 3 for the case where n is a multiple of 16. The first column is the run size and the second column is the number of factors obtained by our methods. Those entries marked with an $*$ are given by Proposition 1. The remaining columns of Table 3 give the number of factors obtained by the methods of Ye (1998), Steinberg and

Lin (2006) and Cioppa and Lucas (2007). Table 3 clearly shows that our methods can provide orthogonal Latin hypercubes when other methods cannot be applied. When other methods are applicable, our methods give many more factors than these existing methods with the only exception given by $n = 256$, for which case Steinberg and Lin (2006) found an OLH(256, 248).

4. Nearly Orthogonal and Cascading Latin Hypercubes

The general construction in (1) is very versatile and can also be used to construct nearly orthogonal and cascading Latin hypercubes. Due to space limitation, we omit the discussion on cascading Latin hypercubes and refer the reader to Lin (2008). In what follows, we provide a brief discussion on nearly orthogonal Latin hypercubes; interested readers can find more details in Lin's thesis (2008).

To assess near orthogonality, we adopt two measures defined in Bingham, Sitter and Tang (2009). For a design $D = (d_1, \dots, d_m)$, where d_j is the j th column of D , define $\rho_{ij}(D)$ to be $d_i^T d_j / [d_i^T d_i d_j^T d_j]^{1/2}$. If the mean of the level settings in d_j for all $j = 1, \dots, m$ is zero, then $\rho_{ij}(D)$ is simply the correlation coefficient between columns d_i and d_j . Near orthogonality can be measured by the maximum correlation $\rho_M(D) = \max_{i,j} |\rho_{ij}(D)|$ and the average squared correlation $\rho^2(D) = \sum_{i < j} \rho_{ij}^2(D) / [(m(m-1)/2)]$. Smaller values of $\rho_M(D)$ and $\rho^2(D)$ imply near orthogonality. Obviously, if $\rho_M(D) = 0$ or $\rho^2(D) = 0$, then an orthogonal Latin hypercube is obtained. The following result shows how the method in (1) can be used to construct nearly orthogonal Latin hypercubes.

Proposition 4. *Suppose that A, B, C, D and γ in (1) are chosen according to Lemma 1 so that design L in (1) is a Latin hypercube. In addition, we assume that A and D are orthogonal and that at least one of the two, $A^T C = 0$ and $B^T D = 0$, holds true. We then have that*

$$(i) \quad \rho^2(L) = w_1 \rho^2(B) + w_2 \rho^2(C), \text{ and}$$

$$(ii) \quad \rho_M(L) = \text{Max}\{w_3 \rho_M(B), w_4 \rho_M(C)\},$$

where w_1, w_2, w_3 and w_4 are given by $w_1 = (m_2 - 1)(n_2^2 - 1)^2 / [(m_1 m_2 - 1)(n^2 - 1)^2]$, $w_2 = n_2^4 (m_1 - 1)(n_1^2 - 1)^2 / [(m_1 m_2 - 1)(n^2 - 1)^2]$, $w_3 = (n_2^2 - 1) / (n^2 - 1)$ and $w_4 = n_2^2 (n_1^2 - 1) / (n^2 - 1)$.

The proof for Proposition 4 is in Appendix A. Proposition 4 says that if B and C are nearly orthogonal, the resulting Latin hypercube L is also nearly orthogonal. An example, illustrating the use of this result, is considered below.

Example 4. Let $A = (1, 1)^T$, $C = (1/2, -1/2)^T$, and $\gamma = 16$. Choose a 16×15 nearly orthogonal Latin hypercube

$$B = \frac{1}{2} \begin{pmatrix} -15 & 15 & -13 & 13 & -5 & -13 & 5 & 3 & -1 & 5 & -7 & 5 & -9 & -9 & 5 \\ -13 & -15 & -3 & 3 & 7 & 3 & 15 & -11 & 13 & -5 & 7 & -13 & -7 & -3 & -3 \\ -11 & -9 & -5 & -11 & -15 & 13 & -5 & 11 & -9 & 9 & 9 & 3 & -5 & -1 & -11 \\ -9 & -1 & 9 & -15 & -11 & 1 & -1 & -13 & 5 & -1 & -15 & 7 & 1 & 3 & 15 \\ -7 & 1 & -7 & 7 & 15 & 15 & -13 & 9 & -5 & -13 & -3 & -1 & -1 & 7 & 13 \\ -5 & 13 & 11 & -5 & 9 & -7 & -3 & -9 & -13 & 11 & 13 & -9 & -3 & 13 & 1 \\ -3 & -5 & 13 & 15 & -9 & -9 & -11 & 1 & 7 & -9 & 15 & 11 & 9 & 1 & -1 \\ -1 & -11 & 3 & -7 & 11 & -15 & 13 & 15 & -7 & -3 & -9 & 9 & 7 & 9 & -5 \\ 1 & 3 & -9 & -3 & -1 & -5 & -15 & -1 & 11 & 3 & -11 & -15 & 15 & 5 & -15 \\ 3 & -3 & 15 & 11 & 3 & 9 & 1 & -7 & -15 & 1 & -13 & -3 & 3 & -15 & -9 \\ 5 & 9 & 7 & -1 & 5 & 11 & 9 & 13 & 15 & 15 & 5 & 1 & 11 & -7 & 9 \\ 7 & 7 & -1 & -13 & 13 & -1 & -7 & -5 & 9 & -7 & 3 & 15 & -13 & -11 & -13 \\ 9 & 5 & -11 & -9 & -7 & -3 & 7 & -3 & -11 & -15 & 11 & -7 & 13 & -13 & 7 \\ 11 & 11 & 5 & 5 & -13 & 7 & 11 & 5 & 3 & -11 & -5 & -5 & -11 & 15 & -7 \\ 13 & -7 & -15 & 9 & 1 & 5 & 3 & -15 & -3 & 13 & 1 & 13 & 5 & 11 & 3 \\ 15 & -13 & 1 & 1 & -3 & -11 & -9 & 7 & 1 & 7 & -1 & -11 & -15 & -5 & 11 \end{pmatrix},$$

which has $\rho^2(B) = 0.0003$ and $\rho_M(B) = 0.0765$. Taking any 15 columns of a Hadamard matrix of order 16 to be D and then applying (1), we obtain a Latin hypercube L of 32 runs and 15 factors. As $\rho^2(C) = \rho_M(C) = 0$, we have $\rho^2(L) = (n_2^2 - 1)^2 \rho^2(B) / (n^2 - 1)^2 = 0.0621 \rho^2(B) = 0.00002$ and $\rho_M(L) = (n_2^2 - 1) \rho_M(B) / (n^2 - 1) = 0.2493 \rho_M(B) = 0.0191$.

A more general result than Proposition 4 can be obtained if A and D are nearly orthogonal and at least one of the two, $A^T C = 0$ and $B^T D = 0$, approximately holds. However, besides being very complicated, such a general result does not greatly enhance our capability of constructing nearly orthogonal Latin hypercubes as the orthogonality of A and D and that between A and C is much easier to achieve than the orthogonality of B and C . Our result as in Proposition 4 makes a more focused presentation. Lin (2008) also contains a table of small nearly orthogonal Latin hypercubes, based on which we can construct large nearly orthogonal Latin hypercubes via Proposition 4.

5. Concluding Remarks

We have presented a general method of construction for orthogonal, nearly orthogonal and cascading Latin hypercubes. The method uses small designs to build large designs. It turns out that some appealing properties in small designs can be carried over to large designs. We have also obtained a result on the existence of orthogonal Latin hypercubes. The power of the general method is further enhanced by the methods of stacking. Although our methods are motivated by computer experiments, they are potentially useful for constructing other designs such as permutation arrays, which are widely applied to data transmission over power lines (Colbourn, Kløve, and Ling (2004) and the reference therein).

Many researchers are increasingly interested in using polynomial models for computer experiments though Gaussian process models are still very popular. Polynomials are attractive because they allow gradual building of a suitable model by starting with simple linear terms and then gradually introducing higher-order terms. Orthogonal and nearly orthogonal Latin hypercubes are directly useful when polynomial models are considered. If one insists on using Gaussian-process models, orthogonality and near orthogonality can be viewed as stepping stones to space-filling designs. This is because a good space-filling design must be orthogonal or nearly so as the design points when projected on to two dimensions should be uniformly scattered. Thus, the search for space-filling designs can be restricted to orthogonal and nearly orthogonal designs instead of all designs. A rich class of orthogonal and nearly orthogonal Latin hypercubes can be obtained by considering a generalization of the construction method in this paper. The generalization makes use of an idea in Bingham, Sitter and Tang (2009); for more details, we refer to Lin (2008). It is part of our research plan to write a paper on this topic in the future.

Acknowledgement

The research is supported by grants from the Natural Sciences and Engineering Research Council of Canada. The authors thank the Associate Editor and referees for their helpful comments.

Appendix A

Proof of Lemma 1. We provide a proof under (a) in condition (ii) of Lemma 1. The proof is essentially the same if condition (b) is met. For design L in (1) to be a Latin hypercube, we need to show that each column of L is a permutation of $-(n-1)/2, -(n-3)/2, \dots, (n-3)/2, (n-1)/2$, where $n = n_1 n_2$. Without loss of generality, we will prove that this is the case for the first column of design L . For ease in notation, let $(a_1, \dots, a_{n_1})^T$, $(b_1, \dots, b_{n_2})^T$, $(c_1, \dots, c_{n_1})^T$ and $(d_1, \dots, d_{n_2})^T$ be the first columns of A , B , C and D , respectively. Then the entries of the first column of L are given by

$$a_i b_j + n_2 c_i d_j, \quad \text{where } i = 1, \dots, n_1 \text{ and } j = 1, \dots, n_2. \quad (8)$$

As C is a Latin hypercube, we have that c_1, \dots, c_{n_1} are a permutation of $-(n_1 - 1)/2, -(n_1 - 3)/2, \dots, (n_1 - 3)/2, (n_1 - 1)/2$. For any given odd u such that $1 \leq u \leq n_1$, consider the two distinct levels, $-(n_1 - u)/2$ and $(n_1 - u)/2$, of C . (The two levels may be the same level 0 when n_1 is odd. This simple case will be dealt with later.) For this given u , let i and i' be the unique indices such that $c_i = (n_1 - u)/2$ and $c_{i'} = -(n_1 - u)/2$. As $d_j = \pm 1$, the two numbers $c_i d_j$ and $c_{i'} d_j$ must always have opposite signs and thus always give the two points $-(n_1 - u)/2$ and $(n_1 - u)/2$ on the real line. Therefore, the two numbers $n_2 c_i d_j$ and $n_2 c_{i'} d_j$ always give the two points $-n_2(n_1 - u)/2$ and $n_2(n_1 - u)/2$ for any $j = 1, \dots, n_2$. By condition (a), we have that $a_i = a_{i'}$. Since B is a Latin hypercube of n_2 runs, we have that b_1, \dots, b_{n_2} are a permutation of $-(n_2 - 1)/2, -(n_2 - 3)/2, (n_2 - 3)/2, (n_2 - 1)/2$. As $a_i = \pm 1$, we have that $a_i b_1, \dots, a_i b_{n_2}$ are also a permutation of $-(n_2 - 1)/2, -(n_2 - 3)/2, (n_2 - 3)/2, (n_2 - 1)/2$. Since $a_{i'} = a_i$, this shows that the $2n_2$ points given by $a_i b_j + n_2 c_i d_j$ and $a_{i'} b_j + n_2 c_{i'} d_j$ for $j = 1, \dots, n_2$ can be divided into two sets of n_2 points with the first set of n_2 points given by $-n_2(n_1 - u)/2 + b_j$ for $j = 1, \dots, n_2$ and the second set of n_2 points given by $n_2(n_1 - u)/2 + b_j$ for $j = 1, \dots, n_2$. The n_2 points $-n_2(n_1 - u)/2 + b_j$ for $j = 1, \dots, n_2$ are centered at $-n_2(n_1 - u)/2$, and equally spaced with two adjacent points separated by an interval of length one. A similar remark can be made about the other set of n_2 points. We note that if $u = n_1$ when n_1 is odd, for the unique i with $c_i = 0$, the n_2 numbers $a_i b_j + n_2 c_i d_j = a_i b_j$ for $j = 1, \dots, n_2$ are simply the set of b_j 's for $j = 1, \dots, n_2$. By allowing the odd u to vary in the range $1 \leq u \leq n_1$, we see that the $n_1 n_2$

numbers in (8) are precisely these n points, $-(n-1)/2, -(n-3)/2, \dots, (n-3)/2, (n-1)/2$, where $n = n_1 n_2$. The proof is completed.

Proof of Theorem 2. The sufficiency part of Theorem 2 can be proved directly, which involves the construction of an orthogonal Latin hypercube of n runs with $m \geq 2$ factors for any n that does not have form $4k+2$. We omit this part of the proof as the existence result also follows from Proposition 3 in Section 3.3 when we establish a lower bound on the maximum number of factors in an orthogonal Latin hypercube.

It remains to show that there does not exist an orthogonal Latin hypercube of $n = 4k+2$ runs with $m \geq 2$ factors. Now suppose that such an orthogonal Latin hypercube exists and let $a = (a_1, \dots, a_n)^T$ and $b = (b_1, \dots, b_n)^T$ be its two columns. Then we have that both a and b are permutations of $\{1/2, 3/2, \dots, (n-1)/2, -1/2, -3/2, \dots, -(n-1)/2\}$. Note that $\sum_{i=1}^n a_i = 0$, $\sum_{i=1}^n b_i = 0$. Without loss of generality, we assume that $a = (1/2, 3/2, \dots, (n-1)/2, -1/2, -3/2, \dots, -(n-1)/2)^T$. In other words, we have $a_i = -a_{i+n/2} = (2i-1)/2$. Since a and b are orthogonal, we have that $\sum_{i=1}^n a_i b_i = 2^{-1} \sum_{i=1}^{n/2} [(2b_i)i - (2b_{i+n/2})(i-1)] = 0$. Note that both $2b_i$ and $2b_{i+n/2}$ are odd, $i = 1, \dots, n/2$. The quantity $(2b_i)i - (2b_{i+n/2})(i-1)$ must be odd as $(2b_i)i$ and $(2b_{i+n/2})(i-1)$ cannot be both even or both odd. In addition, $n/2$ must be odd. It is obvious that the addition or subtraction among an odd number of odd integers gives an odd integer. This leads to a contradiction.

Proof of Proposition 4. Parts (i) and (ii) can be obtained by noting that

$$\begin{aligned} L^T L &= (A \otimes B + \gamma C \otimes D)^T (A \otimes B + \gamma C \otimes D) \\ &= (A^T A) \otimes (B^T B) + \gamma (A^T C) \otimes (B^T D) + \gamma (C^T A) \otimes (D^T B) + \gamma^2 (C^T C) \otimes (D^T D) \\ &= n_1 I_{m_1} \otimes (B^T B) + n_2^2 (C^T C) \otimes (n_2 I_{m_2}), \end{aligned}$$

where I_{m_1} and I_{m_2} are identity matrices of size m_1 and m_2 , respectively. The second step follows by the properties of Kronecker product given in (4). The last step is due to the orthogonality of A and D , either of the conditions $A^T C = 0$ and $B^T D = 0$, and $\gamma = n_2$. In addition, for an $n \times m$ Latin hypercube L , the sum of squares of the elements in each of its columns is $n(n^2-1)/12$. Thus, the $m \times m$ correlation matrix among the m columns of L is given by $[n(n^2-1)/12]^{-1} L^T L$. Based on the elements in the correlation matrix, $\rho^2(L)$ and $\rho_M(L)$ can be computed in the following way,

$$\begin{aligned}\rho^2(L) &= \frac{m_1 n_1^2 m_2 (m_2 - 1) [n_2 (n_2^2 - 1) / 12]^2 \rho^2(B) + n_2^6 m_2 m_1 (m_1 - 1) [n_1 (n_1^2 - 1) / 12]^2 \rho^2(C)}{m_1 m_2 (m_1 m_2 - 1) [n (n^2 - 1) / 12]^2} \\ &= \frac{(m_2 - 1) (n_2^2 - 1)^2 \rho^2(B) + n_2^4 (m_1 - 1) (n_1^2 - 1)^2 \rho^2(C)}{(m_1 m_2 - 1) (n^2 - 1)^2},\end{aligned}$$

and $\rho_m(L) = \text{Max}\{n_1 n_2 [(n_2^2 - 1) / 12] \rho_M(B) / [n (n^2 - 1) / 12], n_2^3 n_1 [(n_1^2 - 1) / 12] \rho_M(C) / [n (n^2 - 1) / 12]\}$. With the definition of w_1, w_2, w_3 and w_4 , we complete the proof.

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