

# Construction of Marginally Coupled Designs by Subspace Theory

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## Abstract

Recent researches on designs for computer experiments with both qualitative and quantitative factors have advocated the use of marginally coupled designs. This paper proposes a general method of constructing such designs for which the designs for qualitative factors are multi-level orthogonal arrays and the designs for quantitative factors are Latin hypercubes with desirable space-filling properties. Two cases are introduced for which we can obtain the guaranteed low-dimensional space-filling property for quantitative factors. Theoretical results on the proposed constructions are derived. For practical use, some constructed designs for three-level qualitative factors are tabulated.

*Key words and phrases:* Cascading Latin hypercube, computer experiment, Latin hypercube, lower-dimensional projection, orthogonal array.

## 1 Introduction

Computer experiments with both qualitative and quantitative variables are becoming increasingly common (see, for example, Rawlingson et al., 2006; Qian, Wu and

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Wu, 2008; Han et al., 2009; Zhou, Qian and Zhou, 2011; Deng et al., 2017). Extensive studies have been devoted to design and modeling of such experiments. This article focuses on a particular class of designs, namely, *marginally coupled designs*, which have been argued to be a cost-effective design choice (Deng, Hung and Lin, 2015). The goal here is to propose a general method for constructing marginally coupled designs when the design for qualitative variables is a multi-level orthogonal array.

The first systematical plan to accommodate computer experiments with both qualitative and quantitative variables is sliced Latin hypercube designs proposed by Qian and Wu (2009). In such a design, for each level combination of the qualitative factors, the corresponding design for the quantitative factor is a small Latin hypercube (McKay, Beckman and Conover, 1979). The run size of a sliced Latin hypercube design increases dramatically with the number of the qualitative factors. To accommodate a large number of qualitative factors with an economical run size, Deng, Hung and Lin (2005) introduced marginally coupled designs which possess the property that with respect to each level of each qualitative variable, the corresponding design for quantitative variables is a sliced Latin hypercube design. Other enhancements of sliced Latin hypercubes include multi-layer sliced Latin hypercube designs (Xie et al., 2014), clustered-sliced Latin hypercube designs (Huang et al., 2016), bi-directional sliced Latin hypercube designs (Zhou et al., 2016).

Since being introduced by Deng, Hung and Lin (2015), there have been two developments of marginally coupled designs, due to He, Lin and Sun (2017) and He et al. (2017), respectively. Comparing with the original work, both developments provide designs for quantitative factors without clustered points, thereby improving the space-filling property which refers to spreading out points in the design region as evenly as possible (Lin and Tang, 2015). He, Lin and Sun (2017) constructs marginally coupled designs of  $s^u$  runs that can accommodate  $(s + 1 - k)s^{u-2}$  qualitative factors and  $k$  quantitative factors for a prime power  $s$  and  $1 \leq k < s + 1$ . The drawback of this method is when  $s = 2$ , the corresponding designs can accommodate only up to 3

quantitative factors. He et al. (2017) addressed this issue and introduced a method for constructing marginally coupled designs of  $2^u$  runs for  $2^{u_1-1}$  qualitative factors of two levels and up to  $2^{u-u_1}$  quantitative factors, where  $1 \leq u_1 \leq u$ .

The paper aims to construct marginally coupled designs of  $s^u$  runs in which designs for qualitative factors are  $s$ -level orthogonal arrays for a prime power  $s$  and any positive integer  $u$ . The primary technique in the proposed construction is the subspace theory of Galois field  $GF(s^u)$ . Although such a technique was used in the constructions in He et al. (2017) for  $s = 2$ , it is not trivial to generalize their constructions for any prime power  $s$ . Extra care must be taken in the generalization. The other contribution of this article is to introduce two cases for which guaranteed low-dimensional space-filling property for quantitative factors can be obtained. For example, for  $s = 2$ , the designs of  $2^u$  runs for quantitative factors achieve stratification on a  $2 \times 2 \times 2$  grid of any three dimensions.

The remainder is arranged as follows. Section 2 introduces background and preliminary results. New constructions and the associated theoretical results are presented in Section 3. Section 4 tabulates the designs with three-level qualitative factors. The space-filling property of the newly constructed designs is discussed in Section 5, and the last section concludes the paper. All the proofs are relegated to Appendix.

## 2 Background and Preliminary Results

### 2.1 Background

A matrix of size  $n \times m$ , where the  $j$ th column has  $s_j$  levels  $0, \dots, s_j - 1$ , is called an orthogonal array of strength  $t$ , if for any  $n \times t$  sub-array, all possible level combinations appear equally often. It is denoted by  $OA(n, s_1 \cdots s_m, t)$  and the simplified notation  $OA(n, s_1^{u_1} s_2^{u_2} \cdots s_k^{u_k}, t)$  will be used if the first  $u_1$  columns have  $s_1$  levels, the next  $u_2$  columns have  $s_2$  levels, and so on. If  $s_1 = \cdots = s_m = s$ , it is shortened as

$OA(n, m, s, t)$ . If all rows of an  $OA(n, m, s, t)$  can form a vector space, it is called a linear orthogonal array (Hedayat, Sloane and Stufken, 1999). For a prime power  $s$ , let  $GF(s) = \{\alpha_0, \alpha_1, \dots, \alpha_{s-1}\}$  be a Galois field of order  $s$ , where  $\alpha_0 = 0$  and  $\alpha_1 = 1$ . Throughout this paper, unless otherwise specified, entries of any  $s$ -level array are from  $GF(s)$ . For a set  $S$ ,  $|S|$  represents the number of elements in  $S$ .

A Latin hypercube is an  $n \times k$  matrix each column of which is a random permutation of  $n$  equally spaced levels (McKay, Beckman and Conover, 1979). In this article, these  $n$  levels are represented by  $0, \dots, n-1$ , and a Latin hypercube of  $n$  runs for  $k$  factors is denoted by  $LHD(n, k)$ . A special type of Latin hypercubes is a *cascading Latin hypercube* for which with  $n = n_1 n_2$  points and levels  $(n_1, n_2)$  is an  $n_2$ -point Latin hypercube about each point in the  $n_1$ -point Latin hypercube (Handcock, 1991). Latin hypercubes can be obtained from orthogonal arrays. Given an  $OA(n, m, s, t)$ , replace the  $r = n/s$  positions having level  $i$  by a random permutation of  $\{ir, \dots, (i+1)r-1\}$ , for  $i = 0, \dots, s-1$ . The resulting design achieves  $t$ -dimensional stratification, and is called an orthogonal array-based Latin hypercube (Tang, 1993). This approach is referred to as the *level replacement-based Latin hypercube* approach.

Let  $D_1$  be an  $OA(n, m, s, 2)$  and  $D_2$  be an  $LHD(n, k)$ . Design  $D = (D_1, D_2)$  is called a *marginally coupled design*, denoted by  $MCD(D_1, D_2)$ , if for each level of every column of  $D_1$ , the corresponding rows in  $D_2$  have the property that when projected onto each column, the resulting entries consist of exactly one level from each of the  $n/s$  equally-spaced intervals  $\{[0, s-1], [s, 2s-1], \dots, [n-s, n-1]\}$ . As a space-filling design is generally sought, a  $D_2$  in which the whole design or any of its column-wise projections has clustered points shall be avoided. We define a Latin hypercube  $D_2$  to be *non-cascading* if, when projected onto any two distinct columns of  $D_2$ , the resulting design is not a cascading Latin hypercube of levels  $(s, n/s)$ .

To study the existence of  $MCD(D_1, D_2)$ 's, He, Lin and Sun (2017) defined the matrix  $\tilde{D}_2$  based on  $D_2$ . Let  $d_{2,ij}$  be the  $(i, j)$ th entry of  $D_2$ . The  $(i, j)$ th entry  $\tilde{d}_{2,ij}$  is given

by

$$\tilde{d}_{2,ij} = \lfloor d_{2,ij}/s \rfloor, \quad i = 1, \dots, n \text{ and } j = 1, \dots, k, \quad (1)$$

where  $\lfloor x \rfloor$  denotes the greatest integer less than or equal to  $x$ . The operator in (1) scales the levels in the interval  $[0, s - 1]$  to level 0, the levels in the interval  $[s, 2s - 1]$  to level 1, and so on. Thus, the levels in  $\tilde{D}_2$  are  $\{0, 1, \dots, n/s - 1\}$ . On the other hand, design  $D_2$  can be obtained from  $\tilde{D}_2$  via the *level replacement-based Latin hypercube* approach. Lemma 1 given by He, Lin and Sun (2017) provides a necessary and sufficient condition for the existence of an  $\text{MCD}(D_1, D_2)$  when  $D_1$  is an  $s$ -level orthogonal array.

**Lemma 1.** *Given that  $D_1$  is an  $\text{OA}(n, m, s, 2)$ ,  $D_2$  is an  $\text{LHD}(n, k)$  and  $\tilde{D}_2$  is defined via (1), then  $(D_1, D_2)$  is a marginally coupled design if and only if for  $j = 1, \dots, k$ ,  $(D_1, \mathbf{d}_j)$  is an  $\text{OA}(n, s^m(n/s), 2)$ , where  $\mathbf{d}_j$  is the  $j$ th column of  $\tilde{D}_2$ .*

In addition to conveniently study the existence of marginally coupled designs, the definition of  $\tilde{D}_2$  allows us to determine whether or not  $D_2$  is *non-cascading*. By definition, a Latin hypercube  $D_2$  is *non-cascading* if any two distinct columns of the corresponding  $\tilde{D}_2$  cannot be transformed to each other by level permutations.

## 2.2 Preliminary results

This subsection presents a result that is the cornerstone of the proposed general construction in next section. Although the result itself is trivial, it is important to review the notation, concepts and existing results to help understand the later development. An example is also given to facilitate the understanding. Suppose that we wish to construct an  $\text{MCD}(D_1, D_2)$  with  $D_1 = \text{OA}(s^u, m, s, 2)$  and  $D_2 = \text{LHD}(s^u, k)$ . Lemma 1 indicates that it is equivalent to construct  $D_1 = (\mathbf{a}_1, \dots, \mathbf{a}_m)$  and  $\tilde{D}_2 = (\mathbf{d}_1, \dots, \mathbf{d}_k) = \text{OA}(s^u, k, s^{u-1}, 1)$  such that  $(\mathbf{d}_j, \mathbf{a}_i) = \text{OA}(s^u, s^{u-1} \times s, 2)$  (Here  $s^{u-1} \times s$  means  $\mathbf{d}_j$  has  $s^{u-1}$  levels, and  $\mathbf{a}_i$  has  $s$  levels) and any distinct two columns  $\mathbf{d}_i$  and  $\mathbf{d}_j$  cannot be transformed to each other by level permutations. This subsection focuses on a construction of an  $\text{OA}(s^u, s^{u-1} \times s, 2)$ .

First, we review the connection between an  $s^{u-1}$ -level column and a  $(u-1)$ -dimensional subspace of  $GF(s^w)$ , where  $w \geq u-1$ . To see this, note that an  $s^{u-1}$ -level column can be generated by choosing a subarray  $A_0 = \text{OA}(s^w, u-1, s, u-1)$  from a linear  $\text{OA}(s^w, m, s, 2)$ , say  $A$ , and substituting each level combination of these columns by a unique level of  $\{0, 1, \dots, s^{u-1} - 1\}$  in some manner. This procedure is known as the *method of replacement* (Wu and Hamada, 2011). One method to achieve the substitution is  $A_0 \cdot (s^{u-2}, \dots, s, 1)^T$ , where the superscript  $T$  represents the transpose of a matrix or a vector; this is exactly what we adopt in this paper. The  $A_0$ , consisting of  $u-1$  independent columns, can also be generated using all linear combinations of rows of a  $w \times (u-1)$  matrix  $G$ , called the *generator matrix* of  $A_0$  (Hedayat, Sloane and Stufken, 1999). In addition, all linear combinations of columns of  $G$  form a  $(u-1)$ -dimensional vector subspace of  $GF(s^w)$ . Therefore, an  $s^{u-1}$ -level column corresponds to one  $(u-1)$ -dimensional subspace of  $GF(s^w)$ , where  $w \geq u-1$ .

Consider the case of  $w = u$ . Let  $S_u$  consist of  $s$ -level column vectors of length  $u$ , then all of its column vectors form a space of dimension  $u$ . For the detail of vector spaces, refer to Horn and Johnson (2015). For two column vectors  $\mathbf{x}, \mathbf{y} \in S_u$ , if  $\mathbf{x}^T \mathbf{y} = 0$  in  $GF(s)$ , they are said to be orthogonal. For a nonzero element  $\mathbf{x} \in S_u$ , define

$$O(\mathbf{x}) = \{\mathbf{y} \in S_u \mid \mathbf{y}^T \mathbf{x} = 0\}. \quad (2)$$

It can be seen that  $O(\mathbf{x})$  is a  $(u-1)$ -dimensional subspace of  $S_u$ .

Let  $G(\mathbf{x})$  be a  $u \times (u-1)$  matrix consisting of  $u-1$  independent columns of  $O(\mathbf{x})$ . For a vector from  $S_u \setminus O(\mathbf{x})$ , say  $\mathbf{z}$ , all linear combinations of rows of the matrix  $(G(\mathbf{x}), \mathbf{z})$  can generate an  $s^u \times u$  matrix. For ease of presentation, the first  $u-1$  columns and the last column of the resulting matrix are denoted by  $A(\mathbf{x})$  and  $\mathbf{a}$ , respectively. Applying the *method of replacement* to  $A(\mathbf{x})$  yields an  $s^{u-1}$ -level vector, say  $\mathbf{d}$ . Lemma 2 indicates that the  $\mathbf{d}$  and  $\mathbf{a}$  are orthogonal.

**Lemma 2.** For  $\mathbf{d}$  and  $\mathbf{a}$  constructed above, we have that  $(\mathbf{d}, \mathbf{a})$  is an  $\text{OA}(s^u, s^{u-1} \times s, 2)$ .

**Example 1.** For  $s = u = 3$ , we have  $GF(3) = \{0, 1, 2\}$  and  $S_3 = \{(x_1, x_2, x_3)^T \mid x_i \in GF(3), i = 1, 2, 3\}$ . Consider  $\mathbf{x} = (1, 2, 0)^T$ , and we have

$$O(\mathbf{x}) = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \end{pmatrix},$$

and the dimension of  $O(\mathbf{x})$  is 2. Choose two independent columns  $(0, 0, 1)^T$  and  $(1, 1, 0)^T$  from  $O(\mathbf{x})$ , and column-combining them gives  $G(\mathbf{x})$ . For  $\mathbf{z} = (1, 2, 0)^T \in S_3 \setminus O(\mathbf{x})$ ,  $(G(\mathbf{x}), \mathbf{z})$  generates a  $27 \times 3$  matrix  $(A(\mathbf{x}), \mathbf{a})$ , whose transpose is as follows

$$\begin{pmatrix} 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 & 1 & 1 & 1 & 2 & 2 & 2 & 0 & 0 & 0 & 2 & 2 & 2 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

By the method of replacement, let  $\mathbf{d} = A(\mathbf{x}) \cdot (3, 1)^T$ . Then  $(\mathbf{d}, \mathbf{a})$  is an  $OA(27, 9 \times 3, 2)$  whose transpose is

$$\begin{pmatrix} 0 & 3 & 6 & 1 & 4 & 7 & 2 & 5 & 8 & 1 & 4 & 7 & 2 & 5 & 8 & 0 & 3 & 6 & 2 & 5 & 8 & 0 & 3 & 6 & 1 & 4 & 7 \\ 0 & 0 & 0 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

### 3 Construction

This section introduces a general construction and a subspace construction for marginally coupled designs using a set of vectors from  $S_u$ . For each construction, a necessary condition for the set of vectors is given. For the given design parameters  $s, u, u_1$ , two constructions provide marginally coupled designs with different numbers of qualitative factors and quantitative factors. The key results are summarized in Theorems 1 and 2.

In the following constructions, when choosing nonzero vectors  $\mathbf{x}, \mathbf{y}$  from  $S_u$  to construct orthogonal arrays or to construct  $(u - 1)$ -dimensional subspaces  $O(\mathbf{x})$  and  $O(\mathbf{y})$ , we require  $\mathbf{x} \neq \alpha \mathbf{y}$  for any  $\alpha \in GF(s)$ . This is because if  $\mathbf{x} = \alpha \mathbf{y}$  for some  $\alpha \in GF(s)$ ,  $\mathbf{x}$

and  $\mathbf{y}$  generate the columns representing the same factor, and  $O(\mathbf{x})$  and  $O(\mathbf{y})$  actually represent the same  $(u - 1)$ -dimensional subspace.

### 3.1 General construction

Suppose we choose  $m + k$  vectors  $\mathbf{z}_1, \dots, \mathbf{z}_m, \mathbf{x}_1, \dots, \mathbf{x}_k$  from  $S_u$ , such that  $\mathbf{z}_i$  is not in any of  $O(\mathbf{x}_j)$ . We propose the following three-step construction.

Step 1. Obtain  $D_1 = (\mathbf{a}_1, \dots, \mathbf{a}_m)$  by taking all linear combinations of the rows of  $(\mathbf{z}_1, \dots, \mathbf{z}_m)$ , where  $\mathbf{a}_i$  is the  $i$ th column of  $D_1$ ;

Step 2. For each  $\mathbf{x}_j$ , choose  $u - 1$  independent columns from  $O(\mathbf{x}_j)$  in (2) to form a generator matrix  $G(\mathbf{x}_j)$ . Obtain  $A(\mathbf{x}_j)$  by taking all linear combinations of the rows of  $G(\mathbf{x}_j)$ . Apply the *method of replacement* to obtain an  $s^{u-1}$ -level column vector  $\mathbf{d}_j$  from  $A(\mathbf{x}_j)$ . Denote the resulting design by  $\tilde{D}_2 = (\mathbf{d}_1, \dots, \mathbf{d}_k)$ ;

Step 3. Obtain  $D_2$  from  $\tilde{D}_2$  via the *level replacement-based Latin hypercube* approach.

The method of obtaining  $\mathbf{d}_j$  and  $\mathbf{a}_i$  in Steps 1 and 2 in the general construction are essentially the construction in Section 2.2 and thus by Lemma 2,  $(\mathbf{d}_j, \mathbf{a}_i)$  is an  $OA(s^u, s^{u-1} \times s, 2)$ . In addition,  $D_1$  is an  $OA(s^u, m, s, 2)$  and  $D_2$  is an  $LHD(s^u, k)$ . Therefore, the  $(D_1, D_2)$  is a marginally coupled design. The condition of the construction is to have  $\mathbf{z}_i$  not in any of  $O(\mathbf{x}_j)$ . To find such  $\mathbf{z}_i$ 's and  $\mathbf{x}_j$ 's, we consider the set of vectors  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\} \subset S_u$ , where  $\mathbf{e}_i$  is a vector of  $S_u$  with the  $i$ th entry equal to 1 and the other entries equal to 0, and  $1 \leq u_1 \leq u$ . We further define

$$\mathcal{A} = \{\mathbf{x} \in S_u \setminus (\cup_{i=1}^{u_1} O(\mathbf{e}_i)) \mid \text{the first entry of } \mathbf{x} \text{ is } 1\}, \quad (3)$$

where  $O(\cdot)$  is defined in (2). The main result of using  $\mathcal{A}$  and  $\mathbf{e}_i$ 's to construct  $MCD(D_1, D_2)$ 's is provided in Theorem 1. Before presenting the theorem, we describe a result which counts the number of vectors in  $\mathcal{A}$ .

**Lemma 3.** *There are  $n_A = (s - 1)^{u_1 - 1} s^{u - u_1}$  column vectors in  $\mathcal{A}$  in (3).*



The value of  $n_A$  is the number of columns in  $D_1$  or  $D_2$ , as revealed in Theorem 1.

**Theorem 1.** For  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$  defined above,  $\mathcal{A}$  in (3) and  $n_A$  in Lemma 3, if in the general construction we

(i) choose  $\mathbf{z}_i = \mathbf{e}_i$  and  $\mathbf{x}_j \in \mathcal{A}$  for  $1 \leq i \leq u_1$  and  $1 \leq j \leq n_A$ , an  $MCD(D_1, D_2)$  with  $D_1 = OA(s^u, u_1, s, u_1)$ ,  $D_2 = LHD(s^u, n_A)$  can be obtained, or,

(ii) choose  $\mathbf{z}_i \in \mathcal{A}$  and  $\mathbf{x}_j = \mathbf{e}_j$  for  $1 \leq i \leq n_A$  and  $1 \leq j \leq u_1$ , an  $MCD(D_1, D_2)$  with  $D_1 = OA(s^u, n_A, s, 2)$ ,  $D_2 = LHD(s^u, u_1)$  can be obtained,

where both  $D_2$ 's are non-cascading Latin hypercubes.

The design  $D_1$ (or  $D_2$ ) in Theorem 1 (i) (or (ii)) can only accommodate  $u_1 \leq u$  columns. A natural question is whether or not more columns in  $D_1$  (or  $D_2$ ) can be constructed. The answer is positive for  $s = 2$  as shown in He et al. (2017) by choosing some linear combinations of  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$  besides themselves for  $\mathbf{z}_i$ 's (or  $\mathbf{x}_j$ 's). For  $s > 2$ , the answer is still positive, however, there is a price to pay. That is, when more columns of  $D_1$  than those in Theorem 1 are constructed using some linear combinations of  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$  in addition to themselves, the number of columns in  $D_2$  will be less than that in Theorem 1. The reason for paying such cost is quantified in Proposition 1.

**Proposition 1.** For  $s > 2$  and the set  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$  defined above, let  $\mathbf{z} = \sum_{i=1}^{u_1} \lambda_i \mathbf{e}_i$  with at least two nonzero coefficients, where  $\lambda_i \in GF(s)$ . For such  $\mathbf{z}$ 's and  $\mathcal{A}$  in (3), there exists a column vector  $\mathbf{x} \in \mathcal{A}$ , such that  $\mathbf{z} \in O(\mathbf{x})$ .

Proposition 1 shows that, when  $s > 2$ , except  $\{\alpha \mathbf{e}_i \mid \alpha \in GF(s) \setminus \{0\}, i = 1, \dots, u_1\}$ , for any of their other combinations, say  $\mathbf{z}$ , it is impossible that  $\mathbf{z}$  is not in  $O(\mathbf{x})$  for all  $\mathbf{x} \in \mathcal{A}$ . This means if adding  $\mathbf{z}$  for constructing one more column for  $D_1$ , not all the columns in  $\mathcal{A}$  can be used for constructing columns for  $D_2$ . As a compromise, after adding more combinations of  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$  for  $D_1$ , we use a subset  $\{\mathbf{x}_1, \dots, \mathbf{x}_k\} \subset \mathcal{A}$  to construct  $(u - 1)$ -dimensional subspaces  $\{O(\mathbf{x}_1), \dots, O(\mathbf{x}_k)\}$ , where  $k < n_A$ . Next section discusses an approach to find such a subset.

### 3.2 Subspace construction

This subsection introduces an approach to find a proper subset  $\{\mathbf{x}_1, \dots, \mathbf{x}_k\} \subset \mathcal{A}$  and judiciously select some linear combinations  $\mathbf{z} = \lambda_1 \mathbf{e}_1 + \dots + \lambda_{u_1} \mathbf{e}_{u_1}$ , with  $\lambda_j \in GF(s)$ , such that  $\mathbf{z} \in S_u \setminus (\cup_{i=1}^k O(\mathbf{x}_i))$ .

One building block of the proposed approach is some disjoint groups of  $\mathcal{A}$ . To partition  $\mathcal{A}$  into different groups, note that for  $1 \leq j \leq u_1$ , the last  $u - u_1$  entries of  $\mathbf{e}_j$  are zeros and thus the first  $u_1$  entries of  $\mathbf{z}$  and  $\mathbf{x}_i$  determine whether or not  $\mathbf{z}$  is orthogonal to  $\mathbf{x}_i$ . In light of this observation, the partition of  $\mathcal{A}$  is based on the distinct values of the first  $u_1$  entries of vectors in  $\mathcal{A}$ . The proof of Lemma 3 reveals that the first  $u_1$  entries of  $\mathbf{x} \in \mathcal{A}$  can take  $n_B = (s - 1)^{u_1 - 1}$  distinct values, say  $\{(1, b_{i2}, \dots, b_{iu_1}) \mid i = 1, \dots, n_B\}$ . Let  $\mathbf{b}_i = (1, b_{i2}, \dots, b_{iu_1}, 0, \dots, 0)^T$ , and define  $\mathcal{A}_i$  to be the subset of  $\mathcal{A}$  whose column vectors have the same first  $u_1$  entries as those of  $\mathbf{b}_i$ . It shall be noted that  $|\mathcal{A}_i| = s^{u - u_1}$  and  $\mathcal{A}_i$ 's form a disjoint partition of  $\mathcal{A}$ . That is,

$$\mathcal{A} = \cup_{i=1}^{n_B} \mathcal{A}_i.$$

The other building block is a set of  $\overline{E}_i$ 's defined as follows. Let  $E = \{\sum_{j=1}^{u_1} \lambda_j \mathbf{e}_j \mid \lambda_j \in GF(s)\}$  consist of all linear combinations of  $\mathbf{e}_1, \dots, \mathbf{e}_{u_1}$ . For fixed  $i$ ,  $\mathbf{b}_i$  and  $\mathcal{A}_i$ ,  $1 \leq i \leq n_B$ , define

$$E_i = \{ \mathbf{z} \in E \mid \mathbf{z}^T \mathbf{b}_i = 0 \} \text{ and } \overline{E}_i = E \setminus E_i.$$

If  $\mathbf{z} \in \overline{E}_i$ , then  $\mathbf{z} \notin O(\mathbf{b}_i)$ , which implies  $\mathbf{z} \notin O(\mathbf{x})$  for all  $\mathbf{x} \in \mathcal{A}_i$  since the last  $u - u_1$  entries of  $\mathbf{z}$  are zeros. This leads to Lemma 4.

**Lemma 4.** *For  $1 \leq v \leq n_B$ , any  $\mathbf{z} \in \cap_{i=1}^v \overline{E}_i$  and any  $\mathbf{x} \in \cup_{i=1}^v \mathcal{A}_i$ , we have  $\mathbf{z} \notin O(\mathbf{x})$ .*

Lemma 4 is useful because it provides  $\{\mathbf{z}_i\}$ 's and  $\{\mathbf{x}_j\}$ 's required by the general construction in Section 3.1. That is, one can choose  $\mathbf{z}_i$  from  $\cap_{i=1}^v \overline{E}_i$ , and  $\mathbf{x}_j$  from  $\cup_{i=1}^v \mathcal{A}_i$ , that is exactly the method Theorem 2 adopts.

So far, it remains to resolve the question that what the elements are in  $\cap_{i=1}^v \overline{E}_i$  for  $1 \leq v \leq n_B$ . The answer is not difficult for  $v = 1$ , and that for  $v = n_B$  can

be found in Proposition 6 in Appendix for interested readers. For  $1 < v < n_B$ , the explicit form for elements in  $\cap_{i=1}^v \overline{E}_i$  depends on the specific sets  $\overline{E}_1, \dots, \overline{E}_v$ . Thus, we cannot express the elements in  $\cap_{i=1}^v \overline{E}_i$  using a general form. However, we are able to compute the number of elements in  $\cap_{i=1}^v \overline{E}_i$  for some cases. Theorem 2 shows that this number is closely related to the number of variables in the marginally coupled design. In practice, experimenters also hope to know the number in advance, as it can help them determine which marginally coupled design to choose given the numbers of qualitative and quantitative variables in the experiment. Proposition 2 below provides the number,  $|\cap_{i=1}^v \overline{E}_i|$ , in some circumstances.

**Proposition 2.** *For  $\{\mathbf{b}_1, \dots, \mathbf{b}_{n_B}\}$  defined above, suppose that there exists a subset  $\{\mathbf{b}_{i_1}, \dots, \mathbf{b}_{i_{n^*}}\}$  such that any  $u_1$  elements of the set are independent, for  $n^* \leq n_B$ . We have that for  $1 \leq v \leq n^*$  and  $1 \leq i_1 < i_2 \dots < i_v \leq n_B$ , the set  $\cap_{j=1}^v \overline{E}_{i_j}$  contains  $f(v)$  elements with*

$$f(v) = \begin{cases} (s-1)^v s^{u_1-v}, & 1 \leq v \leq u_1, \\ m^*, & u_1 + 1 \leq v \leq n^*, \end{cases} \quad (4)$$

where  $m^* = s^{u_1} [1 - \binom{v}{1} s^{-1} + \dots + (-1)^{u_1} \binom{v}{u_1} s^{-u_1}] + \sum_{i=u_1+1}^v (-1)^i \binom{v}{i}$ .

The value of  $n^*$  in Proposition 2 will be studied in Section 3.3. Example 2 provides an illustration of the  $\mathbf{b}_i$ 's,  $\mathcal{A}_i$ 's,  $\overline{E}_i$ 's and Proposition 2.

**Example 2.** *Consider  $s = 3$ ,  $u = 4$  and  $u_1 = 3$ . By definition, we have  $\mathbf{e}_1 = (1, 0, 0, 0)^T$ ,  $\mathbf{e}_2 = (0, 1, 0, 0)^T$  and  $\mathbf{e}_3 = (0, 0, 1, 0)^T$ ,  $\mathcal{A} = \{(x_1, x_2, x_3, x_4)^T \mid x_1 = 1, x_2, x_3 \in \{1, 2\}, x_4 \in \{0, 1, 2\}\}$ ,  $n_B = (3-1)^{3-1} = 4$ ,  $\mathbf{b}_1 = (1, 1, 1, 0)^T$ ,  $\mathbf{b}_2 = (1, 1, 2, 0)^T$ ,  $\mathbf{b}_3 = (1, 2, 1, 0)^T$ , and  $\mathbf{b}_4 = (1, 2, 2, 0)^T$ . The disjoint groups  $\mathcal{A}_1, \dots, \mathcal{A}_4$  are displayed in Table 1. Note that any three of  $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4\}$  are independent. According to (4), we have  $f(1) = 18$ ,  $f(2) = 12$ ,  $f(3) = 8$  and  $f(4) = 6$ . That is, each of  $\overline{E}_i$ 's has 18 vectors, as shown in Table 2; the intersection of any two of  $\overline{E}_i$ 's has 12 vectors, the intersection of any three of  $\overline{E}_i$ 's has 8 vectors, and the intersection of four of them has 6 vectors.*

Table 1: Partition of  $\mathcal{A}$  in Example 2

$\mathcal{A}_1$	$\mathcal{A}_2$	$\mathcal{A}_3$	$\mathcal{A}_4$
1 1 1	1 1 1	1 1 1	1 1 1
1 1 1	1 1 1	2 2 2	2 2 2
1 1 1	2 2 2	1 1 1	2 2 2
0 1 2	0 1 2	0 1 2	0 1 2

Next, we show how to use  $\mathbf{b}_i$ ,  $\mathcal{A}_i$  and  $\overline{E}_i$  ( $i = 1, \dots, n_B$ ) to construct marginally coupled designs. To do so, we define  $E_v^*$ ,  $\mathcal{A}_v^*$  and  $g(v)$  as follows. To define  $E_v^*$ , given  $s$ ,  $u$  and  $u_1$ , find a set of  $\{\mathbf{b}_{i_1}, \dots, \mathbf{b}_{i_{n^*}}\}$ , by calculation or computer search, such that any  $u_1$  elements in the set are independent; for  $1 \leq v \leq n^*$ , obtain  $\cap_{j=1}^v \overline{E}_{i_j}$  which has  $f(v)$  elements as shown in Proposition 2. Define  $E_v^*$  to be the subset of  $\cap_{j=1}^v \overline{E}_{i_j}$  in which the first nonzero entry of each element is equal to 1. The value  $g(v) = f(v)/(s-1)$  is the number of elements of  $E_v^*$ . Define  $\mathcal{A}_v^* = \cup_{j=1}^v \mathcal{A}_{i_j}$ .

**Theorem 2.** For  $E_v^*$ ,  $\mathcal{A}_v^*$  and  $g(v)$  defined above, if in the general construction, we

- (i) choose  $\mathbf{z}_i \in E_v^*$  and  $\mathbf{x}_j \in \mathcal{A}_v^*$ ,  $i = 1, \dots, g(v)$  and  $j = 1, \dots, vs^{u-u_1}$ , an  $MCD(D_1, D_2)$  with  $D_1 = OA(s^u, g(v), s, 2)$ ,  $D_2 = LHD(s^u, vs^{u-u_1})$  can be obtained, or
- (ii) choose  $\mathbf{z}_i \in \mathcal{A}_v^*$  and  $\mathbf{x}_j \in E_v^*$ ,  $i = 1, \dots, vs^{u-u_1}$  and  $j = 1, \dots, g(v)$ , an  $MCD(D_1, D_2)$  with  $D_1 = OA(s^u, vs^{u-u_1}, s, 2)$ ,  $D_2 = LHD(s^u, g(v))$  can be obtained,

where both  $D_2$ 's are non-cascading Latin hypercubes.

For ease of the presentation, the method in Theorem 2 is called *subspace construction*. Example 3 provides a detailed illustration of obtaining marginally coupled designs via the subspace construction using the  $\mathcal{A}_i$ 's and  $\overline{E}_i$ 's in Example 2.

**Example 3.** (Continuation of Example 2) Table 3 presents  $MCD(D_1, D_2)$ 's obtained according to the subspace construction method by choosing  $v = 1, 2, 3$  or 4. As an illustration, we provide the detailed steps of applying item (i) of Theorem 2 for  $v = 3$ . Consider the sets  $\cap_{j=1}^3 \overline{E}_j$  and  $\cup_{j=1}^3 \mathcal{A}_j$ . In Step 1,  $f(3) = 8$ , hence  $g(3) = 4$ . The

Table 2: Vectors of  $\overline{E}_i$ 's in Example 2

$\overline{E}_1$																
0	0	0	1	1	1	1	1	1	0	0	0	2	2	2	2	2
0	1	1	0	0	1	2	1	2	0	2	2	0	0	2	1	2
1	0	1	0	1	0	2	2	1	2	0	2	0	2	0	1	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\overline{E}_2$																
0	0	0	1	1	1	1	1	1	0	0	0	2	2	2	2	2
0	1	1	0	0	1	1	2	2	0	2	2	0	0	2	2	1
1	0	2	0	2	0	1	2	1	2	0	1	0	1	0	2	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\overline{E}_3$																
0	0	0	1	1	1	1	1	1	0	0	0	2	2	2	2	2
0	1	1	0	0	2	1	2	1	0	2	2	0	0	1	2	1
1	0	2	0	1	0	1	2	2	2	0	1	0	2	0	2	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\overline{E}_4$																
0	0	0	1	1	1	1	1	1	0	0	0	2	2	2	2	2
0	1	1	0	0	2	1	1	2	0	2	2	0	0	1	2	1
1	0	1	0	2	0	1	2	1	2	0	2	0	1	0	2	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

four elements in  $\cap_{j=1}^3 \overline{E}_j$  with the first nonzero entry being 1 are  $\mathbf{z}_1 = (0, 0, 1, 0)^T$ ,  $\mathbf{z}_2 = (0, 1, 0, 0)^T$ ,  $\mathbf{z}_3 = (1, 0, 0, 0)^T$ , and  $\mathbf{z}_4 = (1, 2, 2, 0)^T$ ; take  $(\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \mathbf{z}_4)$  as a generator matrix to obtain  $D_1 = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$ , an  $OA(81, 4, 3, 2)$ . In Step 2, the  $3 \cdot 3^{4-3} = 9$  elements in  $\cup_{j=1}^3 \mathcal{A}_j = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_9\}$  are shown in Table 1. For each  $\mathbf{x}_i$ , let  $G(\mathbf{x}_i)$  consist of three independent columns of  $O(\mathbf{x}_i)$ , and take  $G(\mathbf{x}_i)$  as a generator matrix to obtain the matrix  $A_i$ , an  $OA(81, 3, 3, 3)$ ; let  $\mathbf{d}_i = A_i \cdot (3^2, 3, 1)^T$ , and further let  $\tilde{D}_2 = (\mathbf{d}_1, \dots, \mathbf{d}_9)$ , an  $OA(81, 9, 27, 1)$ . In Step 3, construct  $D_2$ , an  $LHD(81, 9)$ , from  $\tilde{D}_2$  by the level-replacement based Latin hypercube approach. The above three-step procedure results in an  $MCD(D_1, D_2)$ , which is listed in Table 3 marked by #, and in the middle of Table 6 marked by  $\diamond$ .

Table 3:  $MCD(D_1, D_2)$ 's with  $s = 3$ ,  $u = 4$  and  $u_1 = 3$  in Example 3

$v$	By item (i)		By item (ii)	
	$D_1$	$D_2$	$D_1$	$D_2$
1	OA(3 <sup>4</sup> , 9, 3, 2)	LHD(3 <sup>4</sup> , 3)	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 9)
2	OA(3 <sup>4</sup> , 6, 3, 2)	LHD(3 <sup>4</sup> , 6)	OA(3 <sup>4</sup> , 6, 3, 2)	LHD(3 <sup>4</sup> , 6)
#3	OA(3 <sup>4</sup> , 4, 3, 2)	LHD(3 <sup>4</sup> , 9)	OA(3 <sup>4</sup> , 9, 3, 2)	LHD(3 <sup>4</sup> , 4)
4	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 12)	OA(3 <sup>4</sup> , 12, 3, 2)	LHD(3 <sup>4</sup> , 3)

### 3.3 The maximum value of $n^*$

Both Proposition 2 and Theorem 2 require a set of vectors  $\{\mathbf{b}_{i_1}, \dots, \mathbf{b}_{i_{n^*}}\}$  in which any  $u_1$  elements are independent. The value of  $n^*$  directly determines the number of columns in  $D_1$  or  $D_2$ . Of theoretical interest is the maximum value of  $n^*$  that can be achieved, and the bound of such a value if not obtained explicitly. We provide the maximum value of  $n^*$  for the three cases: (1)  $s = 2$  with  $u_1 \geq 2$ , (2)  $s > 2$  with  $u_1 = 1$ , and (3)  $s > 2$  with  $u_2 = 2$ . For other values of  $s$ ,  $u$ , and  $u_1$ , we provide bounds of the maximum value of  $n^*$ .

#### Case 1: $s = 2$ , $u_1 \geq 2$

For  $s = 2$ , and  $1 \leq u_1 < u$ , we have  $n_B = (s - 1)^{u_1 - 1} = 1$  and thus  $n^* = 1$ . The only choice for  $\mathbf{b}_i$ 's,  $\mathcal{A}_i$ 's and  $\overline{E}_i$ 's is  $\mathbf{b}_1 = (1, \dots, 1, 0, \dots, 0)$ ,  $\mathcal{A} = \mathcal{A}_1 = \{(1, \dots, 1, x_{u_1+1}, \dots, x_u) \mid x_i \in \{0, 1\}\}$ , and  $\overline{E}_1$  contains all the combinations of  $\lambda_1 \mathbf{e}_1 + \dots + \lambda_{u_1} \mathbf{e}_{u_1}$  that are not orthogonal to column vectors of  $\mathcal{A}_1$ . Note that  $\overline{E}_1$  consists of all combinations with odd numbers of  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u_1}\}$ . Therefore,  $\overline{E}_1$  has  $2^{u_1 - 1}$  elements. In addition,  $v = 1$ ,  $f(1) = g(1) = 2^{u_1 - 1}$  and  $k = 1 \cdot 2^{u - u_1}$ .

#### Case 2: $s \geq 3$ , $u_1 = 1$

As  $u_1 = 1$ , we have  $n_B = (s - 1)^{u_1 - 1} = 1$  and  $n^* = 1$ . It is clear that  $\mathcal{A} = \mathcal{A}_1$ ,  $\overline{E}_1 = \{\alpha \mathbf{e}_1 \mid \alpha \in GF(s) \setminus \{0\}\}$ ,  $v = 1$ ,  $f(1) = s - 1$ ,  $g(1) = 1$  and  $k = 1 \cdot s^{u - 1}$ .

#### Case 3: $s \geq 3$ , $u_1 = 2$

We have  $n_B = (s - 1)^{u_1 - 1} = s - 1$ . The first  $u_1$  entries of vectors of  $\mathcal{A}$  have  $s - 1$

Table 4: Maximum values of  $n^*$  and  $MCD(D_1, D_2)$ 's for  $s = 2$  or  $u_1 \leq 2$

$s$	$u_1$	maximum value of $n^*$	$v$	$g(v)$	$D_1$	$D_2$
$s = 2$	$2 \leq u_1 \leq u$	1	1	$2^{u_1-1}$	$OA(2^u, 2^{u_1-1}, 2, 3)$	$LHD(2^u, 2^{u-u_1})$
			1	$2^{u_1-1}$	$OA(2^u, 2^{u-u_1}, 2, 3)$	$LHD(2^u, 2^{u_1-1})$
$s \geq 3$	1	1	1	1	$OA(s^u, 1, s, 2)$	$LHD(s^u, s^{u-1})$
			1	1	$OA(s^u, s^{u-1}, s, 2)$	$LHD(s^u, 1)$
$s \geq 3$	2	$s-1$	1	$s$	$OA(s^u, s, s, 2)$	$LHD(s^u, s^{u-2})$
			1	$s$	$OA(s^u, s^{u-2}, s, 2)$	$LHD(s^u, s)$
			2	$s-1$	$OA(s^u, s-1, s, 2)$	$LHD(s^u, 2s^{u-2})$
			2	$s-1$	$OA(s^u, 2s^{u-2}, s, 2)$	$LHD(s^u, s-1)$
			$2 < v \leq s-1$	$s-v+1$	$OA(s^u, s-v+1, s, 2)$	$LHD(s^u, vs^{u-2})$
			$2 < v \leq s-1$	$s-v+1$	$OA(s^u, vs^{u-2}, s, 2)$	$LHD(s^u, s-v+1)$

choices as  $(1, \alpha_1)^T, (1, \alpha_2)^T, \dots, (1, \alpha_{s-1})^T$  for  $\alpha_i \in GF(s)$ , hence  $\mathbf{b}_i = (1, \alpha_i, 0, \dots, 0)^T$ . As any two vectors of  $\{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_{s-1}\}$  are independent, the maximum value of  $n^*$  is  $s-1$ . The values of  $f(v)$  at  $v = 1, 2$ , and  $2 < v \leq s-1$  are  $s(s-1)$ ,  $(s-1)^2$  and  $(s-1)(s-v+1)$  according to (4), respectively. The values of  $g(v)$  at  $v = 1, 2$ , and  $2 < v \leq s-1$  are  $s, s-1$  and  $s-v+1$ , respectively.

Table 4 summarizes the maximum values of  $n^*$  under cases 1 to 3, where the marginally coupled designs are obtained as in Theorem 2. For  $s = 2$ ,  $D_1$  is an orthogonal array of strength three follows by Corollary 2 of Deng, Hung and Lin (2015). For  $s, u_1 > 2$ , Proposition 3 presents a bound for the maximum value of  $n^*$ .

**Proposition 3.** *Given positive integers  $s, u > 2$ , and  $2 < u_1 \leq u$ , suppose any  $u_1$  vectors of  $\{\mathbf{b}_1, \dots, \mathbf{b}_{n^*}\}$  are independent. We have*

$$\max n^* \leq \begin{cases} u_1 + 1, & s \leq u_1, \\ s + u_1 - 2, & s > u_1 \geq 3 \text{ and } s \text{ is odd,} \\ s + u_1 - 1, & \text{in all other cases.} \end{cases} \quad (5)$$

**Remark 1.** According to the proof of Proposition 3, the maximum value of  $n^*$  is not greater than the maximum value of  $m$  in an  $OA(s^{u_1}, m, s, u_1)$ . It shall be noted that, however, it is possible to give an upper bound tighter than that given by Proposition

Table 5:  $MCD(D_1, D_2)$ s with  $3^u$  runs by Theorem 1,  $u = 2, 3, 4, 5$

$u$	$u_1$	$n_A$	By item (i)		By item (ii)	
			$D_1$	$D_2$	$D_1$	$D_2$
2	1	3	OA( $3^2, 1, 3, 1$ )	LHD( $3^2, 3$ )	OA( $3^2, 3, 3, 2$ )	LHD( $3^2, 1$ )
2	2	2	OA( $3^2, 2, 3, 2$ )	LHD( $3^2, 2$ )	OA( $3^2, 2, 3, 2$ )	LHD( $3^2, 2$ )
3	1	9	OA( $3^3, 1, 3, 1$ )	LHD( $3^3, 9$ )	OA( $3^3, 9, 3, 2$ )	LHD( $3^3, 1$ )
3	2	6	OA( $3^3, 2, 3, 2$ )	LHD( $3^3, 6$ )	OA( $3^3, 6, 3, 2$ )	LHD( $3^3, 2$ )
3	3	4	OA( $3^3, 3, 3, 3$ )	LHD( $3^3, 4$ )	OA( $3^3, 4, 3, 2$ )	LHD( $3^3, 3$ )
4	1	27	OA( $3^4, 1, 3, 1$ )	LHD( $3^4, 27$ )	OA( $3^4, 27, 3, 2$ )	LHD( $3^4, 1$ )
4	2	18	OA( $3^4, 2, 3, 2$ )	LHD( $3^4, 18$ )	OA( $3^4, 18, 3, 2$ )	LHD( $3^4, 2$ )
4	3	12	OA( $3^4, 3, 3, 3$ )	LHD( $3^4, 12$ )	OA( $3^4, 12, 3, 2$ )	LHD( $3^4, 3$ )
4	4	8	OA( $3^4, 4, 3, 4$ )	LHD( $3^4, 8$ )	OA( $3^4, 8, 3, 2$ )	LHD( $3^4, 4$ )
5	1	81	OA( $3^5, 1, 3, 1$ )	LHD( $3^5, 81$ )	OA( $3^5, 81, 3, 2$ )	LHD( $3^5, 1$ )
5	2	54	OA( $3^5, 2, 3, 2$ )	LHD( $3^5, 54$ )	OA( $3^5, 54, 3, 2$ )	LHD( $3^5, 2$ )
5	3	36	OA( $3^5, 3, 3, 3$ )	LHD( $3^5, 36$ )	OA( $3^5, 36, 3, 2$ )	LHD( $3^5, 3$ )
5	4	24	OA( $3^5, 4, 3, 4$ )	LHD( $3^5, 24$ )	OA( $3^5, 24, 3, 2$ )	LHD( $3^5, 4$ )
5	5	16	OA( $3^5, 5, 3, 5$ )	LHD( $3^5, 16$ )	OA( $3^5, 16, 3, 2$ )	LHD( $3^5, 5$ )

3, for example, for  $u_1 = 2$ , the maximum value of  $n^*$  is  $s - 1$ , but the maximum value of  $m$  in an  $OA(s^2, m, s, 2)$  is  $s + 1$ .

## 4 Tables for Three-level Qualitative Factors

This section tabulates the marginally coupled designs with three-level qualitative factors obtained by the proposed methods for practical use. Tables 5 and 6 present the designs constructed in Theorems 1 and 2, respectively, where  $\bar{u}_1 = u - u_1$ , and the symbol  $*$  indicates the case of  $v = n^*$ .

Since the last  $u - u_1$  entries of each  $\mathbf{b}_i$  are zeros, to obtain the maximum value of  $n^*$ , we only need to consider the independent relationship between the vectors with the first  $u_1$  entries of  $\mathbf{b}_i$ 's. For  $s = 3$ ,  $n_B = 2^{u_1-1}$  and these vectors can form a  $u_1 \times 2^{u_1-1}$  matrix, which is denoted by  $B_{u_1}$  in this paper. Columns of  $B_{u_1}$  are arranged in an order such that the  $j$ th column is determined by the  $(i, j)$ th entry  $B_{u_1}(i, j)$  as follows:

$$j - 1 = \sum_{i=1}^{u_1} 2^{u_1-i} (B_{u_1}(i, j) - 1).$$



Table 6:  $MCD(D_1, D_2)$ s with  $3^u$  runs by Theorem 2,  $u = 2, 3, 4, 5$ 

$u$	$u_1$	$v$	$g(v)$	$\bar{u}_1$	$k$	By item (i)		By item (ii)	
						$D_1$	$D_2$	$D_1$	$D_2$
2	1	1*	1	1	3	OA(3 <sup>2</sup> , 1, 3, 2)	LHD(3 <sup>2</sup> , 3)	OA(3 <sup>2</sup> , 3, 3, 2)	LHD(3 <sup>2</sup> , 1)
2	2	1	3	0	1	OA(3 <sup>2</sup> , 3, 3, 2)	LHD(3 <sup>2</sup> , 1)	OA(3 <sup>2</sup> , 1, 3, 2)	LHD(3 <sup>2</sup> , 3)
2	2	2*	2	0	2	OA(3 <sup>2</sup> , 2, 3, 2)	LHD(3 <sup>2</sup> , 2)	OA(3 <sup>2</sup> , 2, 3, 2)	LHD(3 <sup>2</sup> , 2)
3	1	1*	1	2	9	OA(3 <sup>3</sup> , 1, 3, 2)	LHD(3 <sup>3</sup> , 9)	OA(3 <sup>3</sup> , 9, 3, 2)	LHD(3 <sup>3</sup> , 1)
3	2	1	3	1	3	OA(3 <sup>3</sup> , 3, 3, 2)	LHD(3 <sup>3</sup> , 3)	OA(3 <sup>3</sup> , 3, 3, 2)	LHD(3 <sup>3</sup> , 3)
3	2	2*	2	1	6	OA(3 <sup>3</sup> , 2, 3, 2)	LHD(3 <sup>3</sup> , 6)	OA(3 <sup>3</sup> , 6, 3, 2)	LHD(3 <sup>3</sup> , 2)
3	3	1	9	0	1	OA(3 <sup>3</sup> , 9, 3, 2)	LHD(3 <sup>3</sup> , 1)	OA(3 <sup>3</sup> , 1, 3, 2)	LHD(3 <sup>3</sup> , 9)
3	3	2	6	0	2	OA(3 <sup>3</sup> , 6, 3, 2)	LHD(3 <sup>3</sup> , 2)	OA(3 <sup>3</sup> , 2, 3, 2)	LHD(3 <sup>3</sup> , 6)
3	3	3	4	0	3	OA(3 <sup>3</sup> , 4, 3, 2)	LHD(3 <sup>3</sup> , 3)	OA(3 <sup>3</sup> , 3, 3, 2)	LHD(3 <sup>3</sup> , 4)
3	3	4*	3	0	4	OA(3 <sup>3</sup> , 3, 3, 2)	LHD(3 <sup>3</sup> , 4)	OA(3 <sup>3</sup> , 4, 3, 2)	LHD(3 <sup>3</sup> , 3)
4	1	1*	1	3	27	OA(3 <sup>4</sup> , 1, 3, 2)	LHD(3 <sup>4</sup> , 27)	OA(3 <sup>4</sup> , 27, 3, 2)	LHD(3 <sup>4</sup> , 1)
4	2	1	3	2	9	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 9)	OA(3 <sup>4</sup> , 9, 3, 2)	LHD(3 <sup>4</sup> , 3)
4	2	2*	2	2	18	OA(3 <sup>4</sup> , 2, 3, 2)	LHD(3 <sup>4</sup> , 18)	OA(3 <sup>4</sup> , 18, 3, 2)	LHD(3 <sup>4</sup> , 2)
4	3	1	9	1	3	OA(3 <sup>4</sup> , 9, 3, 2)	LHD(3 <sup>4</sup> , 3)	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 9)
4	3	2	6	1	6	OA(3 <sup>4</sup> , 6, 3, 2)	LHD(3 <sup>4</sup> , 6)	OA(3 <sup>4</sup> , 6, 3, 2)	LHD(3 <sup>4</sup> , 6)
◇4	3	3	4	1	9	OA(3 <sup>4</sup> , 4, 3, 2)	LHD(3 <sup>4</sup> , 9)	OA(3 <sup>4</sup> , 9, 3, 2)	LHD(3 <sup>4</sup> , 4)
4	3	4*	3	1	12	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 12)	OA(3 <sup>4</sup> , 12, 3, 2)	LHD(3 <sup>4</sup> , 3)
4	4	1	27	0	1	OA(3 <sup>4</sup> , 27, 3, 2)	LHD(3 <sup>4</sup> , 1)	OA(3 <sup>4</sup> , 1, 3, 2)	LHD(3 <sup>4</sup> , 27)
4	4	2	18	0	2	OA(3 <sup>4</sup> , 18, 3, 2)	LHD(3 <sup>4</sup> , 2)	OA(3 <sup>4</sup> , 2, 3, 2)	LHD(3 <sup>4</sup> , 18)
4	4	3	12	0	3	OA(3 <sup>4</sup> , 12, 3, 2)	LHD(3 <sup>4</sup> , 3)	OA(3 <sup>4</sup> , 3, 3, 2)	LHD(3 <sup>4</sup> , 12)
4	4	4	8	0	4	OA(3 <sup>4</sup> , 8, 3, 2)	LHD(3 <sup>4</sup> , 4)	OA(3 <sup>4</sup> , 4, 3, 2)	LHD(3 <sup>4</sup> , 8)
4	4	5*	5	0	5	OA(3 <sup>4</sup> , 5, 3, 2)	LHD(3 <sup>4</sup> , 5)	OA(3 <sup>4</sup> , 5, 3, 2)	LHD(3 <sup>4</sup> , 5)
5	1	1*	1	4	81	OA(3 <sup>5</sup> , 1, 3, 2)	LHD(3 <sup>5</sup> , 81)	OA(3 <sup>5</sup> , 81, 3, 2)	LHD(3 <sup>5</sup> , 1)
5	2	1	3	3	27	OA(3 <sup>5</sup> , 3, 3, 2)	LHD(3 <sup>5</sup> , 27)	OA(3 <sup>5</sup> , 27, 3, 2)	LHD(3 <sup>5</sup> , 3)
5	2	2*	2	3	54	OA(3 <sup>5</sup> , 2, 3, 2)	LHD(3 <sup>5</sup> , 54)	OA(3 <sup>5</sup> , 54, 3, 2)	LHD(3 <sup>5</sup> , 2)
5	3	1	9	2	9	OA(3 <sup>5</sup> , 9, 3, 2)	LHD(3 <sup>5</sup> , 9)	OA(3 <sup>5</sup> , 9, 3, 2)	LHD(3 <sup>5</sup> , 9)
5	3	2	6	2	18	OA(3 <sup>5</sup> , 6, 3, 2)	LHD(3 <sup>5</sup> , 18)	OA(3 <sup>5</sup> , 18, 3, 2)	LHD(3 <sup>5</sup> , 6)
5	3	3	4	2	27	OA(3 <sup>5</sup> , 4, 3, 2)	LHD(3 <sup>5</sup> , 27)	OA(3 <sup>5</sup> , 27, 3, 2)	LHD(3 <sup>5</sup> , 4)
5	3	4*	3	2	36	OA(3 <sup>5</sup> , 3, 3, 2)	LHD(3 <sup>5</sup> , 36)	OA(3 <sup>5</sup> , 36, 3, 2)	LHD(3 <sup>5</sup> , 3)
5	4	1	27	1	3	OA(3 <sup>5</sup> , 27, 3, 2)	LHD(3 <sup>5</sup> , 3)	OA(3 <sup>5</sup> , 3, 3, 2)	LHD(3 <sup>5</sup> , 27)
5	4	2	18	1	6	OA(3 <sup>5</sup> , 18, 3, 2)	LHD(3 <sup>5</sup> , 6)	OA(3 <sup>5</sup> , 6, 3, 2)	LHD(3 <sup>5</sup> , 18)
5	4	3	12	1	9	OA(3 <sup>5</sup> , 12, 3, 2)	LHD(3 <sup>5</sup> , 9)	OA(3 <sup>5</sup> , 9, 3, 2)	LHD(3 <sup>5</sup> , 12)
5	4	4	8	1	12	OA(3 <sup>5</sup> , 8, 3, 2)	LHD(3 <sup>5</sup> , 12)	OA(3 <sup>5</sup> , 12, 3, 2)	LHD(3 <sup>5</sup> , 8)
5	4	5*	5	1	15	OA(3 <sup>5</sup> , 5, 3, 2)	LHD(3 <sup>5</sup> , 15)	OA(3 <sup>5</sup> , 15, 3, 2)	LHD(3 <sup>5</sup> , 5)
5	5	1	81	0	1	OA(3 <sup>5</sup> , 81, 3, 2)	LHD(3 <sup>5</sup> , 1)	OA(3 <sup>5</sup> , 1, 3, 2)	LHD(3 <sup>5</sup> , 81)
5	5	2	54	0	2	OA(3 <sup>5</sup> , 54, 3, 2)	LHD(3 <sup>5</sup> , 2)	OA(3 <sup>5</sup> , 2, 3, 2)	LHD(3 <sup>5</sup> , 54)
5	5	3	36	0	3	OA(3 <sup>5</sup> , 36, 3, 2)	LHD(3 <sup>5</sup> , 3)	OA(3 <sup>5</sup> , 3, 3, 2)	LHD(3 <sup>5</sup> , 36)
5	5	4	24	0	4	OA(3 <sup>5</sup> , 24, 3, 2)	LHD(3 <sup>5</sup> , 4)	OA(3 <sup>5</sup> , 4, 3, 2)	LHD(3 <sup>5</sup> , 24)
5	5	5	16	0	5	OA(3 <sup>5</sup> , 16, 3, 2)	LHD(3 <sup>5</sup> , 5)	OA(3 <sup>5</sup> , 5, 3, 2)	LHD(3 <sup>5</sup> , 16)
5	5	6*	11	0	6	OA(3 <sup>5</sup> , 11, 3, 2)	LHD(3 <sup>5</sup> , 6)	OA(3 <sup>5</sup> , 6, 3, 2)	LHD(3 <sup>5</sup> , 11)

Hence the  $j$ th column is labeled by bold  $\mathbf{j} - \mathbf{1}$  in Table 7, in which the matrices of  $B_2$  to  $B_5$  are presented. Correspondingly, define  $B_{u_1}^*$  to be an  $n^*$ -column subset of  $B_{u_1}$ , such that any  $u_1$  columns in it are independent. The following is a list of the sets  $B_2^*$  to  $B_5^*$ :  $B_2^*$  containing columns  $\{\mathbf{0}, \mathbf{1}\}$  of  $B_2$ ;  $B_3^*$  containing columns  $\{\mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{3}\}$  of  $B_3$ ;  $B_4^*$  containing columns  $\{\mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{4}, \mathbf{7}\}$  of  $B_4$ ; and  $B_5^*$  containing columns  $\{\mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{4}, \mathbf{9}, \mathbf{14}\}$  of  $B_5$ , where  $B_2^*$  and  $B_3^*$  are obtained by calculation, and  $B_4^*$  and  $B_5^*$  are obtained by computer search. All of their  $n^*$ 's are maximal, refer to Proposition 3. With those  $B_{u_1}^*$ 's, one can obtain the set of column vectors  $\{\mathbf{b}_{i_1}, \dots, \mathbf{b}_{i_{n^*}}\}$  required by Theorem 2.

Table 7: Matrices  $B_{u_1}$ 's for  $u_1 = 2, 3, 4, 5$  and  $s = 3$

$B_2$		$B_3$				$B_4$									
<b>0</b>	<b>1</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>		
1	1	1	1	1	1	1	1	1	1	1	1	1	1		
1	2	1	1	2	2	1	1	1	1	2	2	2	2		
		1	2	1	2	1	1	2	2	1	1	2	2		
						1	2	1	2	1	2	1	2		
$B_5$															
<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>	<b>11</b>	<b>12</b>	<b>13</b>	<b>14</b>	<b>15</b>
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2
1	1	1	1	2	2	2	2	1	1	1	1	2	2	2	2
1	1	2	2	1	1	2	2	1	1	2	2	1	1	2	2
1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2

## 5 Space-filling Property

One important issue of marginally coupled designs is the space-filling property of design  $D_2$ . To achieve or improve the space-filling property, several approaches have been proposed; see, for example, Dragulic, Santner and Dean (2012), Joseph, Gul and Ba (2015), and Sun and Tang (2017). In our case, one approach to improve the space-filling property is to use an optimal level replacement with some optimization criterion when obtaining  $D_2$  from  $\tilde{D}_2$ , as done in Leary, Bhaskar and Keane (2003); another approach is to make  $D_2$  possess some guaranteed space-filling property, for example,

having uniform projections on lower dimensions. In this paper, we address this issue through the latter approach. For  $s = 2$ , the approach uses a concept, anti-mirror vector, defined below.

**Definition 1.** *Two column vectors  $v_1$  and  $v_2$  of the same length with entries from  $\{0, 1\}$  are said to be anti-mirror vectors if their sum is equal to the vector of all ones. We use the notation  $\bar{v}_1 = v_2$  and  $\bar{v}_2 = v_1$ .*

For example,  $(1, 1, 0)^T$  is the anti-mirror vector of  $(0, 0, 1)^T$ . It is clear that  $v^T \bar{v} = 0$ , and the anti-mirrors of two different vectors are different.

For practical application, given parameters  $1 \leq u_1, u'_1 \leq u$ , item (ii) of Theorem 2 can construct an  $MCD(D_1, D_2)$  with  $D_1 = \text{OA}(2^u, 2^{u-u_1}, 2, 3)$  and  $D_2 = \text{LHD}(2^u, 2^{u_1-1})$ , and item (i) can construct an  $MCD(D_1, D_2)$  with  $D_1 = \text{OA}(2^u, 2^{u'_1-1}, 2, 3)$  and  $D_2 = \text{LHD}(2^u, 2^{u-u'_1})$ . When setting  $u'_1 = u - u_1 + 1$ , the MCD obtained by item (i) has the same set of parameters as that obtained by item (ii). In this sense, for  $s = 2$ , we only need to consider the subspace construction by item (i) of Theorem 2.

To investigate the space-filling property of  $D_2$  when  $D_1$  is a two-level orthogonal array, we take a closer look at Step 2 of the general construction. Recall that  $\mathcal{A} = \mathcal{A}_1$  has  $2^{u-u_1}$  vectors,  $n_B = 1$  and  $\mathbf{b}_1 = (1, \dots, 1, 0, \dots, 0)^T$  with the first  $u_1$  entries being 1. As in item (ii) of Theorem 2, let  $\{\mathbf{x}_1, \dots, \mathbf{x}_{2^{u-u_1}}\}$  be the vectors in  $\mathcal{A}_1$ , and note that each  $\mathbf{x}_i$  can be written as

$$\mathbf{x}_i = (\mathbf{1}_{u_1}^T, \mathbf{y}_i^T)^T,$$

where  $\mathbf{y}_i \neq \mathbf{y}_j$  for  $i \neq j$ . Let  $\mathbf{x}_0 = (1, 1, 0, \dots, 0)^T$  be a vector with the first two entries being 1 and the last  $u_1 - 2$  entries being 0; for  $1 \leq i \leq 2^{u-u_1}$ , define  $\eta_i = (\mathbf{x}_0^T, \bar{\mathbf{y}}_i^T)^T$ , where  $\bar{\mathbf{y}}_i$  is the anti-mirror vector of  $\mathbf{y}_i$ . We have  $\eta_i \in O(\mathbf{x}_i)$  as  $\eta_i^T \mathbf{x}_i = \mathbf{x}_0^T \mathbf{1}_{u_1} + \bar{\mathbf{y}}_i^T \mathbf{y}_i = 0$ . For each  $\mathbf{x}_i$ , let  $G(\mathbf{x}_i)$  be a generator matrix that consists of  $u - 1$  independent columns of  $O(\mathbf{x}_i)$ . Set the first column of  $G(\mathbf{x}_i)$  to be  $\eta_i$ . Generate  $A_i$  based on  $G(\mathbf{x}_i)$  and obtain  $\mathbf{d}_i = A_i \cdot (2^{u-2}, \dots, 2, 1)^T$ , and let  $\tilde{D}_2 = (\mathbf{d}_1, \dots, \mathbf{d}_{2^{u-u_1}})$ . The method is called the *anti-mirror arrangement* in this paper.

**Proposition 4.** *When  $2 \leq u_1 < u - 1$ , the design  $\tilde{D}_2$  obtained by the anti-mirror arrangement is an  $OA(2^u, 2^{u-u_1}, 2^{u-1}, 1)$  achieving stratifications on a  $2 \times 2 \times 2$  grid of any three dimensions.*

For  $s \geq 2$ , Proposition 5 provides a result of the space-filling property of  $D_2$ 's in marginally coupled designs in Theorem 2.

**Proposition 5.** *If the number,  $k$ , of columns in  $D_2$  in Theorem 2 satisfies  $k \leq (s^{u-1} - 1)/(s - 1)$ , a  $\tilde{D}_2$  that achieves stratifications on an  $s \times s$  grid of any two dimensions can be constructed.*

## 6 Conclusion and Discussion

We have proposed a general method for constructing marginally coupled designs of  $s^u$  runs in which the design for quantitative factors is a non-cascading Latin hypercube, where  $s$  is a prime power. The approach uses the theory of  $(u - 1)$ -dimensional subspaces in the Galois field  $GF(s^u)$ . The newly constructed marginally coupled designs with three-level qualitative factors are tabulated. For other prime numbers of levels, marginally coupled designs can be obtained similarly. In addition, we discuss two cases for which guaranteed space-filling property can be obtained.

The results for the subspace construction in this article extend those in He et al. (2017) for two-level qualitative factors to any  $s$ -level qualitative factors. The *Construction 2* of He, Lin and Sun (2017) is also a special case of the general construction in this article. The reason is as follows. There are  $s + 1$  matrices of size  $s^u \times (s^{u-1} - 1)/(s - 1)$ , denoted by  $C_1, \dots, C_{s+1}$ , each of which contains  $s$  replications of the linear saturated orthogonal array  $OA(s^{u-1}, (s^{u-1} - 1)/(s - 1), s, 2)$ . According to their construction procedure, the matrix  $C_i$  is corresponding to the  $(u - 1)$ -dimensional subspace generated by  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u-2}, \mathbf{e}_{u-1} + \alpha_{i-1}\mathbf{e}_u\}$  for  $1 \leq i \leq s$ , and  $C_{s+1}$  is corresponding to the  $(u - 1)$ -dimensional subspace generated by  $\{\mathbf{e}_1, \dots, \mathbf{e}_{u-2}, \mathbf{e}_u\}$ . They are respective-

ly identical to the  $(u - 1)$ -dimensional subspaces  $O(\mathbf{x}_1), \dots, O(\mathbf{x}_{s+1})$ , where  $\mathbf{x}_1 = \mathbf{e}_u$ ,  $\mathbf{x}_i = \mathbf{e}_{u-1} - \alpha_{i-1}^{-1} \mathbf{e}_u$  for  $2 \leq i \leq s$ , and  $\mathbf{x}_{s+1} = \mathbf{e}_{u-1}$ . Therefore, in the general construction, by choosing such  $\mathbf{x}_1, \dots, \mathbf{x}_k$ , for  $1 \leq k < s + 1$ , and choosing  $\mathbf{z}_1, \dots, \mathbf{z}_m$  from the set of  $\cup_{j=k+1}^{s+1} O(\mathbf{x}_j) \setminus (\cup_{i=1}^k O(\mathbf{x}_i))$ , one can obtain the marginally coupled design provided by *Construction 2* of He, Lin and Sun (2017).

For practitioners, three related issues need further investigations. One is that, the low-dimensional projection space-filling property of the quantitative factors for each level of a qualitative factor; the second one is to improve the space-filling property of the quantitative factors in 3 to 4 dimensions, when the two-dimensional uniform projections are already obtained; and the last one is to construct designs with good coverage if perfect space-filling property under some criterion is not expected. We hope to study them and report our results in future.

## Appendix

### *Proof of Lemma 3*

**Proof.** For  $1 \leq i \leq u_1$  and any vector  $\mathbf{x} = (x_1, \dots, x_u)^T \in S_u \setminus O(\mathbf{e}_i)$ , we have  $\mathbf{x}^T \mathbf{e}_i \neq 0$ , that means  $x_i \neq 0$ . Thus, for any  $\mathbf{x} \in \mathcal{A}$ , we have  $x_1 = 1$ ,  $x_i \in GF(s) \setminus \{0\}$  for  $i = 2, \dots, u_1$ , and  $x_j \in GF(s)$  for  $j = u_1 + 1, \dots, u$ . So, the conclusion follows.  $\square$

### *Proof of Theorem 1*

**Proof.** As every  $\mathbf{z}_i$  is not in any of  $O(\mathbf{x}_j)$ , every  $\mathbf{x}_j$  is not in any of  $O(\mathbf{z}_i)$ . The conclusion follows by the definition of  $\mathcal{A}$ , Lemma 2, and Lemma 1. Because in both items (i) and (ii),  $O(\mathbf{x}_i) \neq O(\mathbf{x}_j)$  when  $i \neq j$ ,  $\mathbf{d}_i$  cannot be transformed to  $\mathbf{d}_j$  by level permutations. Thus  $D_2$ 's are non-cascading Latin hypercubes.  $\square$

### *Proof of Proposition 1*

**Proof.** Suppose  $\mathbf{z} = \sum_{i=1}^{u_1} \lambda_i \mathbf{e}_i$  has  $l$  nonzero coefficients  $\lambda_1, \dots, \lambda_l$ , where  $1 \leq i_j \leq u_1$  and  $2 \leq l \leq u_1$ . Denote by  $\lambda^* = \sum_{j=1}^{l-1} \lambda_{i_j}$ , and let  $\mathbf{x} = (x_1, \dots, x_u)^T$ . If  $\lambda^*$  is nonzero, take  $x_{i_l} = -\lambda_{i_l}^{-1} \lambda^*$  and all the other  $x_i$ 's equal 1, then  $\mathbf{x} \in \mathcal{A}$  since the first

$u_1$  entries of  $\mathbf{x}$  are nonzero. More specifically, the first entry of  $\mathbf{x}$  is 1, and

$$\mathbf{z}^T \mathbf{x} = \sum_{i=1}^{u_1} \lambda_i x_i = \sum_{j=1}^l \lambda_{i_j} x_{i_j} = \sum_{j=1}^{l-1} \lambda_{i_j} \cdot 1 + \lambda_{i_l} \cdot x_{i_l} = \lambda^* - \lambda_{i_l} \cdot \lambda_{i_l}^{-1} \lambda^* = 0,$$

where the first equality holds because the last  $u - u_1$  entries of  $\mathbf{z}$  are zeros. Otherwise, if  $\lambda^* = 0$ , we must have  $l - 1 \geq 2$ , and one can take  $x_{i_{l-1}} = \alpha_2$ ,  $x_{i_l} = -\lambda_{i_l}^{-1} \lambda_{i_{l-1}} (\alpha_2 - 1)$ , and all other  $x_i$ 's equal 1. Note for  $s > 2$ , we have  $\alpha_2 \neq 1$ , hence  $x_{i_l} \neq 0$  and  $\mathbf{x} \in \mathcal{A}$  again. In addition,

$$\mathbf{z}^T \mathbf{x} = \sum_{i=1}^{u_1} \lambda_i x_i = \sum_{j=1}^l \lambda_{i_j} x_{i_j} = \sum_{j=1}^{l-1} \lambda_{i_j} \cdot 1 + \lambda_{i_{l-1}} \cdot (\alpha_2 - 1) - \lambda_{i_l} \cdot \lambda_{i_l}^{-1} \lambda_{i_{l-1}} (\alpha_2 - 1) = 0.$$

So, there always exists an  $\mathbf{x} \in \mathcal{A}$ , such that  $\mathbf{z} \in O(\mathbf{x})$ .  $\square$

### *Proof of Proposition 2*

**Proof.** First, consider  $v = 1$ . As  $(\sum_{j=1}^{u_1} \lambda_j e_j)^T \mathbf{b}_1 = 0$ , we have

$$\lambda_1 b_{11} + \lambda_2 b_{12} + \cdots + \lambda_{u_1} b_{1u_1} = 0.$$

There are  $s^{u_1-1}$  solutions for such an equation, hence there are  $s^{u_1} - s^{u_1-1} = (s-1)s^{u_1-1}$  combinations in  $\overline{E}_1$ .

For  $v = 2$ , as  $(\sum_{j=1}^{u_1} \lambda_j e_j)^T \mathbf{b}_i = 0$  for  $i = 1, 2$ , then

$$\begin{cases} \lambda_1 b_{11} + \lambda_2 b_{12} + \cdots + \lambda_{u_1} b_{1u_1} = 0, \\ \lambda_1 b_{21} + \lambda_2 b_{22} + \cdots + \lambda_{u_1} b_{2u_1} = 0, \end{cases}$$

which has  $s^{u_1-2}$  solutions since  $\mathbf{b}_1$  and  $\mathbf{b}_2$  are independent. However, elements in  $\overline{E}_1 \cap \overline{E}_2$  should not be the solution of neither of the two equations. Then, we have

$$|\overline{E}_1 \cap \overline{E}_2| = |E \setminus (E_1 \cup E_2)| = s^{u_1} - \left[ \binom{2}{1} s^{u_1-1} - \binom{2}{2} s^{u_1-2} \right] = (s-1)^2 s^{u_1-2}.$$

For  $1 \leq v \leq u_1$ , as any  $u_1$  elements of  $\{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_{n^*}\}$  are independent, we have

$$\begin{aligned} |\cap_{i=1}^v \overline{E}_i| &= |E \setminus \cup_{i=1}^v E_i| = s^{u_1} - \left[ \binom{v}{1} s^{u_1-1} - \binom{v}{2} s^{u_1-2} + \cdots + (-1)^{v-1} \binom{v}{v} s^{u_1-v} \right] \\ &= s^{u_1} \left[ 1 - \binom{v}{1} s^{-1} + \cdots + (-1)^v \binom{v}{v} s^{-v} \right] \\ &= (s-1)^v s^{u_1-v}. \end{aligned}$$

For  $u_1 + 1 \leq v \leq n^*$ , the intersection of any  $t \geq u_1$  sets of  $E_i$ 's only contains one vector, namely the zero column vector. Since any  $u_1$  elements of  $\{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_{n^*}\}$  are independent, we have

$$\begin{aligned}
|\cap_{i=1}^v \overline{E}_i| &= |E \setminus \cup_{i=1}^v E_i| & (6) \\
&= s^{u_1} - \left[ \binom{v}{1} s^{u_1-1} - \binom{v}{2} s^{u_1-2} + \dots + (-1)^{u_1-1} \binom{v}{u_1} s^{u_1-u_1} \right. \\
&\quad \left. + (-1)^{u_1} \binom{v}{u_1+1} \cdot 1 + \dots + (-1)^{v-1} \binom{v}{v} \cdot 1 \right] \\
&= s^{u_1} \left[ 1 - \binom{v}{1} s^{-1} + \dots + (-1)^{u_1} \binom{v}{u_1} s^{-u_1} \right] + \sum_{i=u_1+1}^v (-1)^i \binom{v}{i} \\
&= m^*.
\end{aligned}$$

□

*Proof of Theorem 2*

**Proof.** Followed by Lemma 4, for any  $\mathbf{z} \in \cap_{j=1}^v \overline{E}_{i_j}$  and  $\mathbf{x} \in \cup_{j=1}^v \mathcal{A}_{i_j}$ , we have  $\mathbf{z} \notin O(\mathbf{x})$ . Thus, by Lemmas 2 and 1, the  $(D_1, D_2)$ 's constructed in both items are marginally coupled designs. In addition, both items (i) and (ii),  $O(\mathbf{x}_i) \neq O(\mathbf{x}_j)$  when  $i \neq j$ , which implies that  $\mathbf{d}_i$  cannot be obtained from  $\mathbf{d}_j$  by level permutations. Therefore,  $D_2$ 's are non-cascading Latin hypercubes. □

*Proof of Proposition 3*

**Proof.** Since any  $u_1$  vectors of  $\{\mathbf{b}_1, \dots, \mathbf{b}_{n^*}\}$  are independent, one can use them to obtain an  $\text{OA}(s^{u_1}, n^*, s, u_1)$ . The run size here is  $s^{u_1}$ , not  $s^u$ , because the last  $u - u_1$  entries of  $\mathbf{b}_i$ 's are zeros. Note that the maximum value of  $n^*$  must not be greater than the maximum value of  $m$  for an  $\text{OA}(s^{u_1}, m, s, u_1)$  to exist. The right hand side of (5) are the upper bounds of  $m$  for different cases, which were provided by Theorem 2.19 of Hedayat, Sloane and Stufken (1999). □

*Proof of Proposition 4*

**Proof.** It is straightforward to see  $\tilde{D}_2$  is an  $\text{OA}(2^u, 2^{u-u_1}, 2^{u-1}, 1)$ . For  $u - u_1 > 1$  and therefore  $2^{u-u_1} > 3$ , consider a subarray  $(\mathbf{d}_p, \mathbf{d}_q, \mathbf{d}_l)$  of  $\tilde{D}_2$ , for  $1 \leq p < q < l \leq 2^{u-u_1}$ . Let  $\mathbf{c}_i = \lfloor \mathbf{d}_i / 2^{u-2} \rfloor$ . As  $\mathbf{d}_i = A_i \cdot (2^{u-2}, \dots, 2, 1)^T$ ,  $\mathbf{c}_i$  is the first column of  $A_i$ . In

addition,  $(\mathbf{c}_p, \mathbf{c}_q, \mathbf{c}_l)$  is the projection of  $(\mathbf{d}_p, \mathbf{d}_q, \mathbf{d}_l)$  on the  $2 \times 2 \times 2$  grid. Because  $A_i$  is constructed by  $G(\mathbf{x}_i)$ ,  $\mathbf{c}_i$  is generated from  $\eta_i$ . As  $\mathbf{y}_i \neq \mathbf{y}_j$  for  $i \neq j$ , we have  $\bar{\mathbf{y}}_i \neq \bar{\mathbf{y}}_j$ . Since the last  $u - u_1$  entries of  $\eta_i$  is  $\bar{\mathbf{y}}_i$ ,  $\eta_p, \eta_q$  and  $\eta_l$  are three different columns. In addition,  $\eta_p + \eta_q \neq \eta_l$  because the first  $u_1$  entries of  $\eta_p, \eta_q, \eta_l$  are equal to  $\mathbf{x}_0 = (1, 1, 0, \dots, 0)^T$ . As a result,  $\eta_p, \eta_q, \eta_l$  are three independent column vectors. Thus, the array  $(\mathbf{c}_p, \mathbf{c}_q, \mathbf{c}_l)$  is an  $OA(2^u, 3, 2, 3)$ , and the conclusion follows.  $\square$

*Proof of Proposition 5*

**Proof.** In the subspace construction of Theorem 2, for  $i = 1, \dots, k$ , each  $O(\mathbf{x}_i)$  contains a set of  $(s^{u-1} - 1)/(s - 1)$  different column vectors, the first nonzero entry of each of which is equal to 1. If  $k \leq (s^{u-1} - 1)/(s - 1)$ , one can always choose  $\mathbf{y}_i \in O(\mathbf{x}_i)$ , such that  $\mathbf{y}_i \neq \alpha \mathbf{y}_j$  for  $1 \leq i \neq j \leq k$  and any  $\alpha \in GF(s)$ . Let  $\mathbf{y}_i$  be the first column of  $G(\mathbf{x}_i)$  which is used to obtain  $A_i$  and consists of  $u - 1$  independent columns of  $O(\mathbf{x}_i)$ . For such  $\{A_1, \dots, A_k\}$ , the first  $k$  columns form an  $OA(s^u, k, s, 2)$ , which guarantees  $\tilde{D}_2$  to achieve stratifications on an  $s \times s$  grid of any two dimensions.  $\square$

**Proposition 6.** *The set  $\cap_{i=1}^{n_B} \bar{E}_i$  is equal to (i)  $\{\mathbf{e}_{i_1} + \mathbf{e}_{i_2} + \dots + \mathbf{e}_{i_{2t+1}} \mid 2t + 1 \leq u_1, 1 \leq i_1 < i_2 < \dots < i_{2t+1} \leq u_1\}$  when  $s = 2$ , or equal to (ii)  $\{\alpha \mathbf{e}_i \mid \alpha \in GF(s) \setminus \{0\}, i = 1, \dots, u_1\}$  when  $s > 2$ .*

**Proof.** For  $s = 2$ , we have  $n_B = 1$ ,  $\mathcal{A} = \mathcal{A}_1$ , and  $\mathbf{b}_1 = (1, \dots, 1, 0, \dots, 0)^T$  where the first  $u_1$  entries are equal to 1. If  $\mathbf{z} \in E$  and  $\mathbf{z}^T \mathbf{b}_1 \neq 0$ ,  $\mathbf{z}$  must be a sum of an odd number of  $\mathbf{e}_i$ 's. Thus, item (i) follows. If  $\mathbf{z} \in \cap_{i=1}^{n_B} \bar{E}_i$ ,  $\mathbf{z} \notin O(\mathbf{x})$  for any  $\mathbf{x} \in \mathcal{A}$  by Lemma 4. Therefore, for  $s > 2$ , the possible elements in  $\cap_{i=1}^{n_B} \bar{E}_i$  can only be  $\mathbf{z} = \alpha \mathbf{e}_j$  for any  $\alpha \in GF(s) \setminus \{0\}$  and  $j = 1, \dots, u_1$ , according to Proposition 1, while  $\mathbf{e}_j \in \cap_{i=1}^{n_B} \bar{E}_i$ , for  $j = 1, \dots, u_1$ . Combining these two results, item (ii) follows.  $\square$



## Acknowledgements

The authors wish to thank the Editor, an Associate Editor, and two referees for their helpful comments which have led to the improvement of the manuscript.

Yuanzhen He is supported by the National Natural Science Foundation of China Grant 11701033. C. Devon Lin's research was supported by the Discovery grant from Natural Sciences and Engineering Research Council of Canada. Fasheng Sun is supported by the National Natural Science Foundation of China Grants 11471069, 11771220 and the Fundamental Research Funds for the Central Universities.

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