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# Marginally coupled designs for two-level qualitative factors



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# ABSTRACT

Computer experiments with qualitative and quantitative factors occur frequently in various applications in science, engineering and business. For choosing input settings of such computer experiments, marginally coupled designs have been proposed in Deng, Hung and Lin (2015) for economic reasons. Although the concept of marginally coupled designs is well understood, the results on design construction are scarce. In addition, the constructed designs may have clustered points for the quantitative factors or cannot accommodate many quantitative factors, especially for two-level qualitative factors. To address this issue, this paper focuses on constructing marginally coupled designs when all qualitative factors have two levels. The proposed construction uses subspace theory in algebra, and the resulting designs can accommodate more quantitative factors while maintaining attractive design properties than the existing approaches.

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# 1. Introduction

Computer experiment is an efficient and cost-effective surrogate of physical experiment to study complex systems. It is not uncommon that computer experiments have both quantitative and qualitative factors (Qian et al., 2008; Han et al., 2009; Zhou et al., 2011). In such experiments, different qualitative factors may have identical or distinct numbers of levels. This article focuses on a special case that all qualitative factors have two levels. For example, in a knee computer model for investigating wear mechanisms of total knee replacements in bioengineering (Han et al., 2009), the qualitative factors are the prosthesis design and the loading pattern, both at two levels. The levels of the prosthesis design are "cruciate retaining" and "posterior stabilized", while the levels of the loading pattern are "the loading corresponding to normal gait" and "the loading corresponding to stair climbing". For reasons of efficiency and economy, orthogonal arrays, also known as fractional factorial designs, are most commonly used in practice for qualitative factors.

For efficiently choosing input settings for computer experiments with both qualitative and quantitative factors, marginally coupled designs proposed by Deng et al. (2015) have been argued to be a cost-effective alternative to the strategic plan, sliced Latin hypercube designs (Qian and Wu, 2009). The construction of such designs have been explored by Deng et al. (2015) and He et al. (2016). The designs for quantitative factors in the former, however, have undesirable clustered points. For a prime power *s*, the latter has developed the characterization for marginally coupled designs of  $s^u$  runs, and the obtained designs for qualitative factors can accommodate as many as  $(s + 1 - k)s^{u-2}$  factors of *s* levels and designs for quantitative factors can hold *k* factors without clustered points, where  $1 \le k \le s$ . Therefore, the latter can only handle up

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to two quantitative factors when qualitative factors are all at two levels. The goal of this article is to introduce a method for constructing marginally coupled designs possessing a moderate number of quantitative factors when all qualitative factors have two levels.

Although the characterization of a marginally coupled design with  $s^{u}$  runs is derived, there is still lack of construction of desirable marginally coupled designs. We present here a new construction for such designs with qualitative factors of two levels. The construction is simple and it is done by introducing a novel use of subspaces of the vector space on Galois field  $GF(2^u)$ , where u is an integer greater than one. Along the way, useful theoretical results are derived. The results allow us to construct marginally coupled designs of  $2^{u}$  runs. In the newly constructed designs, designs for qualitative factors can accommodate up to 2<sup>u1-1</sup> factors and designs for quantitative factors are Latin hypercube designs without clustered points for up to  $2^{u-u_1}$  factors, for  $1 < u_1 < u$ .

The remainder of this paper is organized as follows. Section 2 introduces notation and background, theoretical results and the construction method are presented in Section 3, and the last section concludes the paper with discussions.

#### 2. Notation, definitions and background

A matrix of size  $n \times m$ , where the *j*th column has  $s_i$  levels  $0, \ldots, s_i - 1$  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( $n, s_1 \cdots s_m, t$ ). If  $s_1 = \cdots = s_m = s_n$ 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 et al., 1999).

A Latin hypercube is an  $n \times k$  matrix each column of which is a random permutation of n equally spaced levels (McKay et al., 1979). In this article, these n levels are represented by  $0, \ldots, n-1$ , and a Latin hypercube of n runs for k factors is denoted by LHD(n, k). A cascading Latin hypercube of  $n = n_1 n_2$  points with 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 (Tang, 1993), Given an OA(n, m, s, t), replace the r = n/s positions having level i by a random permutation of  $\{ir, \ldots, (i+1)r-1\}$ , for  $i=0, \ldots, s-1$ . The resulting design achieves t-dimensional uniformity. This approach is referred to as level replacement-based Latin hypercube approach (He et al., 2016).

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  $\{[0, s-1], [s, 2s-1], \dots, [n-s, n-1]\}$ . Let  $D_{2,ij}$  and  $\tilde{D}_{2,ij}$  be the (i, j)th entry of  $D_2$  and  $\tilde{D}_2$ , respectively, and let

$$\tilde{D}_{2,ij} = \left\lfloor D_{2,ij}/s \right\rfloor, \quad i = 1, \dots, n \text{ and } j = 1, \dots, k,$$

$$(1)$$

where  $\lfloor x \rfloor$  denotes the greatest integer less than or equal to x. Design  $D_2$  can be obtained from  $\tilde{D}_2$  via the level replacementbased Latin hypercube approach. Lemma 1, due to He et al. (2016), provides a necessary and sufficient condition for an  $MCD(D_1, D_2)$  when  $D_1$  is an s-level orthogonal array. The result indicates that to construct  $D_2$ , it is equivalent to construct  $\tilde{D}_2$  that satisfies such a condition.

**Lemma 1.** Given that  $D_1$  is an OA(n, m, s, 2),  $D_2$  is an 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, ..., k,  $(D_1, \tilde{d}_i)$  is an  $OA(n, s^m(n/s), 2)$ , where  $\tilde{d}_i$  is the *j*th column of  $\tilde{D}_2$ .

We now review the background on vector spaces which are building blocks of the proposed construction. Define

$$S_2 = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}.$$

A linear combination of rows in the subarray of  $S_2$  without the zero column can be expressed as (2)

$$\lambda_1(1 \ 0 \ 1) + \lambda_2(0 \ 1 \ 1), \quad \lambda_1, \lambda_2 \in GF(2),$$

where  $GF(2) = \{0, 1\}$  and + represents addition by modulus 2, that is, we have 0+0 = 0, 0+1 = 1, 1+0 = 1, and 1+1 = 0. Take all such  $2^2$  linear combinations in (2) as rows of a new array, then the resulting array is a linear OA( $2^2$ , 3, 2, 2). For  $u \ge 3$ ,  $S_u$  is defined inductively as follows,

$$S_u = \begin{pmatrix} S_{u-1} & S_{u-1} \\ 0_{2^{u-1}} & 1_{2^{u-1}} \end{pmatrix},$$
(3)

where  $0_{2^{u-1}}$  and  $1_{2^{u-1}}$  are row vectors of length  $2^{u-1}$ . It can be seen that all columns of  $S_u$  form a vector space of dimension u. In the same fashion as in (2), a linear OA( $2^u$ ,  $2^u - 1$ , 2, 2) can be generated by taking all the combinations of rows of the matrix which is obtained by excluding the column of zeros, which is the first column of  $S_{\mu}$ .

Let x and y be any two column vectors of  $S_u$ . If  $x^T y = 0$  modulus 2, we say x and y are orthogonal, where the superscript T means the transpose. For any nonzero column vector  $x \in S_u$ , let O(x) consist of all those column vectors in  $S_u$  that are orthogonal to x, that is,

$$O(x) = \{ y \in S_u \mid x^T y = 0 \}.$$
<sup>(4)</sup>

(2)

We can see that O(x) in (4) is a (u - 1)-dimensional subspace of  $S_u$ . Denote by N(x) the matrix consisting of all nonzero column vectors of O(x), and construct a new array by taking all row combinations of N(x) as its rows, then the obtained array is a linear  $OA(2^u, 2^{u-1} - 1, 2, 2)$ , which contains two subarrays each of which is an  $OA(2^{u-1}, 2^{u-1} - 1, 2, 2)$ . On the other hand, it is known that a linear  $OA(2^{u-1}, 2^{u-1} - 1, 2, 2)$  can be used to construct a  $2^{u-1}$ -level column vector via the *method of replacement* (Wu and Hamada, 2011). Therefore, one (u-1)-dimensional subspace O(x) can provide one  $2^{u-1}$ -level column vector of length  $2^u$ .

## 3. Construction using subspace theory

This section introduces a new method for constructing marginally coupled designs in which the designs for qualitative factors are orthogonal arrays of two levels. Throughout this paper, let u be an integer greater than one, and  $E_{u_1} = \{e_1, \ldots, e_{u_1}\}$ , where  $e_1, \ldots, e_{u_1}$  are  $u_1$  independent column vectors of  $S_u$ , with  $1 \le u_1 < u$ . Denote by |S| the number of elements in a set S and  $A \setminus B$  the set consisting of elements belonging to A but not B. Before presenting the proposed construction, we provide Lemmas 2–4 which are cornerstones for establishing Theorem 1.

#### Lemma 2. For the set

$$P = \{\xi \mid \xi = e_{i_1} + e_{i_2} + \dots + e_{i_{2t+1}}, 1 \le i_1 < \dots < i_{2t+1} \le u_1, e_{i_j} \in E_{u_1}\},$$
(5)

we have  $|P| = 2^{u_1 - 1}$ .

Since each member of *P* is a sum of an odd number of elements in  $\{e_1, \ldots, e_{u_1}\}$ , Lemma 2 follows directly by the property of binomial coefficients.

**Lemma 3.** For  $S_u$  in (3) with  $u \ge 2$ , we have  $|S_u \setminus \{\bigcup_{i=1}^{u_1} O(e_i)\}| = 2^{u-u_1}$ , where  $1 \le u_1 < u$ ,  $e_i \in E_{u_1}$  and  $O(e_i)$  is defined by (4).

**Proof.** Let  $n^* = |\bigcup_{i=1}^{u_1} O(e_i)|$ . By the inclusion–exclusion principle, we have that

$$n^* = \sum_{1 \le i \le u_1} |O(e_i)| - \sum_{1 \le i < j \le u_1} |O(e_i) \cap O(e_j)| + \dots + (-1)^{u_1 - 1} |O(e_1) \cap O(e_2) \dots \cap O(e_{u_1})|.$$
(6)

Since  $e_1, \ldots, e_{u_1}$  are independent, there are  $2^{u-2}$  column vectors in  $S_u$  which are orthogonal to both  $e_i$  and  $e_j$ , which means  $|O(e_i) \cap O(e_j)| = 2^{u-2}$ ,  $1 \le i < j \le u_1$ ; and there are  $2^{u-p}$  column vectors orthogonal to a set of p distinct independent columns  $\{e_{i_1}, \ldots, e_{i_p}\}, 2 \le p \le u_1$ . Therefore,

$$n^* = \binom{u_1}{1} 2^{u-1} - \binom{u_1}{2} 2^{u-2} + \dots + (-1)^{u_1-1} \binom{u_1}{u_1} 2^{u-u_1} = 2^u - 2^{u-u_1}.$$

Thus,  $|S_u \setminus (\bigcup_{i=1}^{u_1} O(e_i))| = 2^u - (2^u - 2^{u-u_1}) = 2^{u-u_1}$ .  $\Box$ 

**Lemma 4.** For any subset  $S \subset S_u$  and any nonzero column vector  $x \in S_u$ , if S and O(x) are disjoint, where O(x) is defined in (4), we have that (i) there does not exist three vectors  $a, b, c \in S$  such that a + b = c, and (ii) for any set Q in which each element is a sum of an odd number of vectors in S, as

$$Q = \{q = y_1 + y_2 + \dots + y_{2t+1} \mid y_j \in S, 1 \le 2t + 1 \le |S|\},\$$

then  $Q \cap O(x) = \emptyset$ .

**Proof.** For part (i), suppose  $a, b, c \in S$  such that a + b = c. Then  $\{0_u, a, b, c\}$  is a two-dimensional subspace of  $S_u$ , where  $0_u \in S_u$  is a column of all zeros. Since S and O(x) are disjoint, the union  $S \cup O(x)$  must contain 2 + (u - 1) = u + 1 independent columns. This causes a contradiction because  $S \cup O(x)$  is a subset of  $S_u$  whose dimension is only u. Hence, part (i) is proved. For part (ii), consider an element  $q = y_1 + y_2 + \cdots + y_{2t+1} \in Q$ , where  $y_i \in S$ . For any  $y \in S$ , then  $y \notin O(x)$ , that implies  $y^T x = 1$  modulus 2. So  $q^T x = (y_1 + y_2 + \cdots + y_{2t+1})^T x = 2t + 1$  modulus 2, then  $q^T x = 1$ . Hence,  $q \notin O(x)$ , and we have  $Q \cap O(x) = \emptyset$ .

New notation is introduced here. Let  $G_0$  be the  $u \times 2^{u_1-1}$  matrix each column of which is an element of P defined in Lemma 2. Without loss of generality, suppose  $\{e_1, \ldots, e_{u_1}\}$  are the first  $u_1$  columns of  $G_0$ . Each column of  $G_0$  is a linear combination of an odd number of columns among its first  $u_1$  columns. Write  $G_0 = (g_{1,0}^T, \ldots, g_{u,0}^T)^T$ , where  $g_{i,0}$  is the *i*th row of  $G_0$ .

According to Lemma 3, count the set  $S_u \setminus \{\bigcup_{i=1}^{u_1} O(e_i)\}$  by

$$S_{u} \setminus \left\{ \bigcup_{i=1}^{u_{1}} O(e_{i}) \right\} = \{a_{1}, a_{2}, \dots, a_{2^{u-u_{1}}}\}.$$
(7)

For  $j = 1, ..., 2^{u-u_1}$ , let  $G_j$  be the  $u \times (2^{u-1} - 1)$  matrix by taking all nonzero vectors of  $O(a_j)$  as columns, and write  $G_j = (g_{1,j}^T, ..., g_{u,j}^T)^T$ , where  $g_{i,j}$  is the *i*th row of  $G_j$ . We now propose the following procedure to construct designs  $D_1$  and  $\tilde{D}_2$  of  $2^u$  runs.

Step 1. Construct a  $2^{u} \times 2^{u_1-1}$  matrix whose rows are from linear combinations of rows in  $G_0$ , as

 $\lambda_1 g_{1,0} + \lambda_2 g_{2,0} + \cdots + \lambda_u g_{u,0},$ 

where  $\lambda_i \in GF(2)$  for i = 1, ..., u. Denote the constructed array by  $D_1$ . Then  $D_1$  is a linear OA( $2^u, 2^{u_1-1}, 2, 2$ ), referring to the verification for Construction 3 of Rao-Hamming construction, Section 3.4 of Hedayat et al. (1999). Step 2. For  $j = 1, ..., 2^{u-u_1}$ , construct a  $2^u \times (2^{u-1} - 1)$  matrix whose rows are from linear combinations of rows in  $G_i$ , as

$$\lambda_1 g_{1,i} + \lambda_2 g_{2,i} + \cdots + \lambda_u g_{u,i}$$

where  $\lambda_i \in GF(2)$  for i = 1, ..., u. Denote the obtained matrix by  $D_{2,j}$ . Then  $D_{2,j}$  is a linear OA( $2^u, 2^{u-1} - 1, 2, 2$ ) by the same reason stated in Step 1.

Step 3. For  $j = 1, ..., 2^{u-u_1}$ , obtain a vector of length  $2^u$  with  $2^{u-1}$  levels based on  $D_{2,j}$  via the method of replacement, and denote it by  $\tilde{d}_j$ . Let  $\tilde{D}_2 = (\tilde{d}_1, \tilde{d}_2, ..., \tilde{d}_{2^{u-u_1}})$ .

For ease of presentation, the above construction for designs  $D_1$  and  $\tilde{D}_2$  consisting of Steps 1 to 3 is called the subspace method.

**Theorem 1.** For designs  $D_1$  and  $\tilde{D}_2$  constructed by the subspace method, we have that (i)  $D_1$  is an  $OA(2^u, 2^{u_1-1}, 2, 3)$ , (ii)  $\tilde{D}_2$  is an  $OA(2^u, 2^{u-u_1}, 2^{u-1}, 1)$ , and (iii) each column of  $\tilde{D}_2$  is orthogonal to all columns of  $D_1$ .

**Proof.** To show part (i), first note that  $D_1$  is a linear  $OA(2^u, 2^{u_1-1}, 2, 2)$  according to the construction process of Step 1. Next, we should show  $D_1$  in fact is of strength three. It is seen that  $a_1$  in (7) is not in any of  $\{O(e_1), \ldots, O(e_{u_1})\}$ , hence all  $e_1, \ldots, e_{u_1}$  are not in  $O(a_1)$ , implying  $\{e_1, \ldots, e_{u_1}\} \cap O(a_1) = \emptyset$ . Take  $S = \{e_1, \ldots, e_{u_1}\}$ , then by item (ii) of Lemma 4, one can obtain  $P \cap O(a_1) = \emptyset$ , since each member of P is a combination of an odd number of elements in S; and furthermore, no three elements  $a, b, c \in P$  have a + b = c by item (i) of Lemma 4. This ensures any three columns of  $G_0$  are independent, and the strength of  $D_1$  must be three. So,  $D_1$  is an  $OA(2^u, 2^{u_1-1}, 2, 3)$ .

For  $a_j$ 's in (7) and  $j = 1, ..., 2^{u-u_1}$ ,  $O(a_j)$  is a subspace of dimension u - 1. Then the array  $D_{2,j}$  generated from  $G_j$  is a linear OA( $2^u$ ,  $2^{u-1} - 1$ , 2, 2) consisting of two subarrays each of which is an OA( $2^{u-1}$ ,  $2^{u-1} - 1$ , 2, 2), and the resulting  $\tilde{d}_j$  from  $D_{2,j}$  by the method of replacement is a  $2^{u-1}$ -level vector of length  $2^u$ . As a result,  $\tilde{D}_2 = (\tilde{d}_1, \tilde{d}_2, ..., \tilde{d}_{2^{u-u_1}})$  is an OA( $2^u$ ,  $2^{u-u_1}$ ,  $2^{u-1}$ , 1).

For any  $j = 1, ..., 2^{u-u_1}$ , we have  $P \cap O(a_j) = \emptyset$  according to item (ii) of Lemma 4, which means each column of  $G_0$  is independent to  $G_i$ , hence each column of  $D_1$  is independent to  $D_{2,j}$ , and thus orthogonal to  $\tilde{d}_j$ .  $\Box$ 

For  $D_1$  and  $\tilde{D}_2$  constructed by the subspace method, let  $D_2$  be an LHD $(2^u, 2^{u-u_1})$  obtained from  $\tilde{D}_2$  via the level replacement-based Latin hypercube approach. The following corollary presents the property of  $(D_1, D_2)$  constructed by the subspace method.

**Corollary 1.** We have that (i) design  $(D_1, D_2)$  is a marginally coupled design, and (ii)  $D_2$  is not a cascading Latin hypercube.

**Proof.** By Lemma 1 and Theorem 1, the conclusion of item (i) is direct. For item (ii),  $O(a_i)$  and  $O(a_j)$  present different (u-1)-dimensional subspaces when  $i \neq j$ , thus the resulting  $\tilde{d}_i$  and  $\tilde{d}_j$  are not isomorphic to each other, meaning that one of them cannot be obtained from the other by level permutations, which yields that  $D_2$  is not a cascading Latin hypercube.  $\Box$ 

Example 1 illustrates the proposed construction method.

**Example 1.** Consider u = 4 and  $u_1 = 3$ . The  $S_4$  is defined in (3). Let  $e_1 = (1, 0, 0, 0)^T$ ,  $e_2 = (0, 1, 0, 0)^T$  and  $e_3 = (0, 0, 1, 0)^T$ . Then  $P = \{e_1, e_2, e_3, e_1 + e_2 + e_3\}$ . There are  $2^{u-u_1} = 2$  column vectors in  $S_4 \setminus \{O(e_1) \cup O(e_2) \cup O(e_3)\}$ , named by  $a_1$  and  $a_2$ , which are  $(1, 1, 1, 0)^T$  and  $(1, 1, 1, 1)^T$ , respectively. The subspaces  $O(a_1)$  and  $O(a_2)$  are listed in Table 1. Then matrix  $G_0 = (e_1, e_2, e_3, e_1 + e_2 + e_3)$ , and matrices  $G_1$  and  $G_2$  take all nonzero column vectors of  $O(a_1)$  and  $O(a_2)$  as their columns, respectively.

According to the subspace method, by Step 1, obtain  $D_1$  by including all linear combinations of rows in  $G_0$ ; by Step 2, construct  $D_{2,i}$  by including all linear combinations of rows in  $G_i$ , for i = 1, 2; by Step 3, construct  $\tilde{d}_i$  from  $D_{2,i}$  for i = 1, 2; and obtain  $\tilde{D}_2 = (\tilde{d}_1, \tilde{d}_2)$ . For saving space, the obtained  $D_1$  and  $\tilde{D}_2$  are shown in their transposes in Table 2. One can obtain  $D_2$  from  $\tilde{D}_2$  via the level replacement-based Latin hypercube approach. The resulting  $(D_1, D_2)$  is a marginally coupled design with  $D_2$  being a non-cascading Latin hypercube according to Corollary 1.

In practice, it is desirable that design  $D_2$  in an MCD $(D_1, D_2)$  possesses some guaranteed space-filling property. In fact, this can be pursued by some proper way of substituting  $D_{2,j}$ 's with  $\tilde{d}_j$ 's. Note that this substitution is done by the method of replacement which transforms a linear OA $(2^{u-1}, 2^{u-1} - 1, 2, 2)$  to a  $2^{u-1}$ -level column vector. The method of replacement is essentially equivalent to choosing u - 1 independent columns from the orthogonal array, and then replace each level combination of the u - 1 columns with a unique level in  $\{0, 1, \ldots, 2^{u-1} - 1\}$ . For illustration, let us revisit Example 1.

<i>a</i> <sub>1</sub>	Subspa	ace $O(a_1)$								
1	0	1	1	0	0	1	1	0		
1	0	1	0	1	0	1	0	1		
1	0	0	1	1	0	0	1	1		
0	0	0	0	0	1	1	1	1		
<i>a</i> <sub>2</sub>	Subspa	Subspace O(a <sub>2</sub> )								
1	0	1	1	1	0	0	0	1		
1	0	1	0	0	1	1	0	1		
1	0	0	1	0	1	0	1	1		
1	0	0	0	1	0	1	1	1		

**Table 1**Two three-dimensional subspaces of  $S_4$  in Example 1.

## Table 2

Designs  $D_1$  and  $\tilde{D}_2$ .

0 1 2															
Transpose of D <sub>1</sub>															
0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
0	0	0	0	1	1	1	1	0	0	0	0	1	1	1	1
0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1
0	0	1	1	1	1	0	0	1	1	0	0	0	0	1	1
Transpose of $\tilde{D}_2$															
0	1	2	3	4	5	6	7	6	7	4	5	2	3	0	1
0	7	2	5	3	4	1	6	6	1	4	3	5	2	7	0

#### Table 3

Marginally coupled designs constructed by the subspace method.

и	<i>u</i> <sub>1</sub>	$D_1$	<i>D</i> <sub>2</sub>
2	1	OA(4, 1, 2, 3)	LHD(4, 2)
3	1	OA(8, 1, 2, 3)	LHD(8, 4)
3	2	OA(8, 2, 2, 3)	LHD(8, 2)
4	1	OA(16, 1, 2, 3)	LHD(16, 8)
4	2	OA(16, 2, 2, 3)	LHD(16, 4)
4	3	OA(16, 4, 2, 3)	LHD(16, 2)
5	1	OA(32, 1, 2, 3)	LHD(32, 16)
5	2	OA(32, 2, 2, 3)	LHD(32, 8)
5	3	OA(32, 4, 2, 3)	LHD(32, 4)
5	4	OA(32, 8, 2, 3)	LHD(32, 2)
6	1	OA(64, 1, 2, 3)	LHD(64, 32)
6	2	OA(64, 2, 2, 3)	LHD(64, 16)
6	3	OA(64, 4, 2, 3)	LHD(64, 8)
6	4	OA(64, 8, 2, 3)	LHD(64, 4)
6	5	OA(64, 16, 2, 3)	LHD(64, 2)
7	1	OA(128, 1, 2, 3)	LHD(128, 64)
7	2	OA(128, 2, 2, 3)	LHD(128, 32)
7	3	OA(128, 4, 2, 3)	LHD(128, 16)
7	4	OA(128, 8, 2, 3)	LHD(128, 8)
7	5	OA(128, 16, 2, 3)	LHD(128, 4)
7	6	OA(128, 32, 2, 3)	LHD(128, 2)

**Example 2** (*Continue* Example 1). In Step 3 of the subspace method, choose a three-column submatrix of  $D_{2,1}$ , denoted by  $(p_1, p_2, p_3)$ , corresponding to column vectors (1, 1, 0, 0), (1, 0, 1, 0) and (0, 0, 0, 1) of  $O(a_1)$ ; in parallel, choose a submatrix of  $D_{2,2}$ , denoted by  $(q_1, q_2, q_3)$ , corresponding to column vectors (1, 0, 0, 1), (1, 1, 1, 1), and (0, 1, 0, 1) of  $O(a_2)$ . Note that  $(p_1, p_2, p_3)$  and  $(q_1, q_2, q_3)$  consist of three independent columns of  $D_{2,1}$  and  $D_{2,2}$ , respectively. The replacement of  $D_{2,i}$ 's to  $\tilde{d}_i$ 's is done by  $\tilde{d}_1 = (p_1, p_2, p_3)r$  and  $\tilde{d}_2 = (q_1, q_2, q_3)r$ , where  $r = (2^2, 2^1, 2^0)^T$ . Since either  $(p_1, q_1, q_2)$  or  $(p_1, p_2, q_1)$  has three independent columns,  $(\tilde{d}_1, \tilde{d}_2)$  possesses uniform stratifications in the 2 × 4 and 4 × 2 grids of the two dimensions, that can be verified by design  $\tilde{D}_2$  in Table 2.

For practical applications, Table 3 lists marginally coupled designs with run sizes up to 128 that can be constructed by the subspace method, where the first two columns are for the parameters u and  $u_1$ , and the last two columns present the design  $D_1$  for the qualitative factors and the non-cascading Latin hypercube design  $D_2$  for the quantitative factors, respectively.

# 4. Discussion

This paper introduces a method to construct marginally coupled designs  $MCD(D_1, D_2)$  with  $D_1$  being an  $OA(2^{u}, 2^{u_1-1}, 2, 3)$  and  $D_2$  being a non-cascading Latin hypercube design of size  $2^{u} \times 2^{u-u_1}$ , for integers u and  $1 < u_1 < u$ .

For qualitative factors of two levels, the Construction 2 in He et al. (2016) can obtain an  $MCD(D_1, D_2)$  with  $D_1$  being an  $OA(2^u, 2^{u-2}, 2, 3)$  and  $D_2$  being a non-cascading Latin hypercube design of size  $2^u \times 2$ . In fact, such pairs of designs can also be obtained by the subspace method.

The link between the subspace method and the Construction 2 of He et al. (2016) can be as follows. Let us first look at the subspace method. To avoid the trivial case, we let  $u \ge 3$ . Then set  $u_1 = u - 1$ ,  $e_1 = (1, 0, ..., 0, 1, 1)^T$ ,  $e_2 = (0, 1, 0, ..., 0, 1, 1)^T$ , and so on  $e_{u-2} = (0, ..., 1, 1, 1)^T$  and  $e_{u-1} = (0, ..., 0, 1, 1)^T$ , such that for  $1 \le i \le u - 2$ , the *i*th and the last two entries of  $e_i$  are ones, and other entries are zeros, and for i = u - 1, only the last two entries of  $e_{u-1}$  are ones. By Lemma 2, one can obtain *P* based on  $\{e_1, ..., e_{u-1}\}$ , then *P* has  $2^{(u-1)-1} = 2^{u-2}$  elements; and by Lemma 3,  $S_u \setminus \{\bigcup_{i=1}^{u-1} O(e_i)\}$  has  $2^{u-(u-1)} = 2$  elements, named by  $a_1$  and  $a_2$ . It can be shown that  $a_1 = (0, ..., 0, 1, 0)^T$  and  $a_1 = (0, ..., 0, 1, 0)^T$  and  $a_2 = (0, \dots, 0, 0, 1)^T$ , with the (u - 1)th entry and the *u*th entry being one, respectively, and other entries being zeros. As such, by the subspace method, one can construct  $D_1$  based on  $G_0$  in Step 1, which is obtained from P, and construct  $D_{2,1}$  and  $D_{2,2}$  based on  $G_1$  and  $G_2$  in Step 2, that are obtained from  $O(a_1)$  and  $O(a_2)$ , respectively.

Recall Construction 2 in He et al. (2016). Suppose  $\tilde{e}_1, \ldots, \tilde{e}_u$  are u independent columns, such that  $(\tilde{e}_1, \ldots, \tilde{e}_u)$  is a full factorial design of  $2^u$  runs. Given  $(\tilde{e}_1, \ldots, \tilde{e}_u)$ , He et al. (2016) constructed the matrices  $B_0$ ,  $B_1$ ,  $B_2$  and  $B_3$  as follows. Matrix  $B_0$ is the saturated design generated by the first u - 2 independent columns  $\{\tilde{e}_1, \ldots, \tilde{e}_{u-2}\}$ ,  $B_1$  is the saturated design generated by u - 1 independent columns as  $\{\tilde{e}_1, \ldots, \tilde{e}_{u-2}, \tilde{e}_{u-1}\}$ ,  $B_2$  is the saturated design generated by u - 1 independent columns as  $\{\tilde{e}_1, \ldots, \tilde{e}_{u-2}, \tilde{e}_{u-1} + \tilde{e}_u\}$ , and  $B_3$  is the saturated design generated by u - 1 independent columns as  $\{\tilde{e}_1, \ldots, \tilde{e}_{u-2}, \tilde{e}_u\}$ . In fact we can find that the matrix  $D_1$  in Step 1 of the subspace method is the matrix  $B_2 \setminus B_0$  in the Construction 2, and the matrices  $D_{2,1}$  and  $D_{2,2}$  in Step 2 of the subspace method are the matrices of  $B_3$  and  $B_1$  in the Construction 2, respectively.

One important issue for marginally coupled designs is the space-filling property of design  $D_2$ . One way to obtain spacefilling  $D_2$  is to employ some optimization strategies with some optimality criterion when constructing  $D_2$  from  $\tilde{D}_2$  via the level-replacement-based Latin hypercube approach (Leary et al., 2003). Another way is to use the scheme that we provide in Example 2. Because of the amount of technical details involved, we do not present the general scheme and its associated results for constructing space-filling  $D_2$  here. The application of subspace theory into a prime power s > 2 is under research.

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