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Construction of marginally coupled designs by subspace theory

YUANZHEN HE[1], C. DEVON LIN[2] and FASHENG SUN[3,4]

[1]*Beijing Normal University, Beijing, China*
[2]*Queen's University, Kingston, Canada*
[3]*KLAS, Changchun, China*
[4]*Northeast Normal University, Changchun, China. E-mail: sunfs359@nenu.edu.cn*

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.

Keywords: 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, Rawlinson et al. [17]; Qian, Wu and Wu [16]; Han et al. [4]; Zhou, Qian and Zhou [23]; Deng et al. [2]). 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 [1]). 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 [15]. 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 [14]). 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 [1] 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. [21]), clustered-sliced Latin hypercube designs (Huang et al. [10]), bi-directional sliced Latin hypercube designs (Zhou et al. [22]).

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Since being introduced by Deng, Hung and Lin [1], there have been two developments of marginally coupled designs, due to He, Lin and Sun [6] and He et al. [7], 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 [13]). He, Lin and Sun [6] 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 $1 \le k < s+1$. The drawback of this method is when $s=2$, the corresponding designs can accommodate only up to 3 quantitative factors. He et al. [7] 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 $1 \le u_1 \le u$.

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. [7] 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 jth 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 [8]). 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 [14]). 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 [5]). Latin hypercubes can be obtained from orthogonal arrays. Given an $\mathrm{OA}(n, m, s, t)$, 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 stratification, and is called an orthogonal array-based Latin hypercube (Tang [19]). This approach is referred to as the *level replacement-based Latin hypercube* approach.

Let D_1 be an $\mathrm{OA}(n, m, s, 2)$ and D_2 be an $\mathrm{LHD}(n, k)$. Design $D = (D_1, D_2)$ is called a *marginally coupled design*, denoted by $\mathrm{MCD}(D_1, D_2)$, 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 $\{[0, s-1], [s, 2s-1], \ldots, [n-s, n-1]\}$. 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 $\mathrm{MCD}(D_1, D_2)$'s, He, Lin and Sun [6] 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

$$\tilde{d}_{2,ij} = \lfloor d_{2,ij}/s \rfloor, \qquad i = 1, \ldots, n \text{ and } j = 1, \ldots, k, \tag{1}$$

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 $\{0, 1, \ldots, n/s - 1\}$. 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 [6] provides a necessary and sufficient condition for the existence of an $\mathrm{MCD}(D_1, D_2)$ when D_1 is an s-level orthogonal array.

Lemma 1. *Given that D_1 is an $\mathrm{OA}(n, m, s, 2)$, D_2 is an $\mathrm{LHD}(n, k)$ and $\tilde{D}_2$ is defined via (1), then (D_1, D_2) is a marginally coupled design if and only if for $j = 1, \ldots, k$, $(D_1, \mathbf{d}_j)$ is an $\mathrm{OA}(n, s^m(n/s), 2)$, where $\mathbf{d}_j$ is the jth 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 $\mathrm{MCD}(D_1, D_2)$ with $D_1 = \mathrm{OA}(s^u, m, s, 2)$ and $D_2 = \mathrm{LHD}(s^u, k)$. Lemma 1 indicates that it is equivalent to construct $D_1 = (\mathbf{a}_1, \ldots, \mathbf{a}_m)$ and $\tilde{D}_2 = (\mathbf{d}_1, \ldots, \mathbf{d}_k) = \mathrm{OA}(s^u, k, s^{u-1}, 1)$ such that $(\mathbf{d}_j, \mathbf{a}_i) =$

$\mathrm{OA}(s^u, s^{u-1} \times s, 2)$ (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 $\mathrm{OA}(s^u, s^{u-1} \times s, 2)$.

First, we review the connection between an s^{u-1}-level column and a $(u-1)$-dimensional subspace of $\mathrm{GF}(s^w)$, where $w \geq u-1$. To see this, note that an s^{u-1}-level column can be generated by choosing a subarray $A_0 = \mathrm{OA}(s^w, u-1, s, u-1)$ from a linear $\mathrm{OA}(s^w, m, s, 2)$, say A, and substituting each level combination of these columns by a unique level of $\{0, 1, \ldots, s^{u-1}-1\}$ in some manner. This procedure is known as the *method of replacement* (Wu and Hamada [20]). One method to achieve the substitution is $A_0 \cdot (s^{u-2}, \ldots, s, 1)^T$, 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 [8]). In addition, all linear combinations of columns of G form a $(u-1)$-dimensional vector subspace of $\mathrm{GF}(s^w)$. Therefore, an s^{u-1}-level column corresponds to one $(u-1)$-dimensional subspace of $\mathrm{GF}(s^w)$, 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 [9]. For two column vectors $\mathbf{x}, \mathbf{y} \in S_u$, if $\mathbf{x}^T\mathbf{y} = 0$ in $\mathrm{GF}(s)$, they are said to be orthogonal. For a nonzero element $\mathbf{x} \in S_u$, define

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

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* $\mathrm{OA}(s^u, s^{u-1} \times s, 2)$.

Example 1. For $s = u = 3$, we have $\mathrm{GF}(3) = \{0, 1, 2\}$ and $S_3 = \{(x_1, x_2, x_3)^T \mid x_i \in \mathrm{GF}(3), i = 1, 2, 3\}$. 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 27×3 matrix $(A(\mathbf{x}), \mathbf{a})$, whose transpose is as follows

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

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

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

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 $\alpha \in \mathrm{GF}(s)$. This is because if $\mathbf{x} = \alpha\mathbf{y}$ for some $\alpha \in \mathrm{GF}(s)$, $\mathbf{x}$ 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 $\mathbf{z}_1, \ldots, \mathbf{z}_m, \mathbf{x}_1, \ldots, \mathbf{x}_k$ 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 $D_1 = (\mathbf{a}_1, \ldots, \mathbf{a}_m)$ by taking all linear combinations of the rows of $(\mathbf{z}_1, \ldots, \mathbf{z}_m)$, where $\mathbf{a}_i$ is the ith 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 $\tilde{D}_2 = (\mathbf{d}_1, \ldots, \mathbf{d}_k)$;

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 $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\} \subset S_u$, where $\mathbf{e}_i$ is a vector of S_u with the ith entry equal to 1 and the other entries equal to 0, and $1 \leq u_1 \leq u$. We further define

$$\mathcal{A} = \left\{ \mathbf{x} \in S_u \setminus \left(\bigcup_{i=1}^{u_1} O(\mathbf{e}_i) \right) \,\middle|\, \text{the first entry of } \mathbf{x} \text{ is } 1 \right\}, \tag{3}$$

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* $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$ *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* $1 \le i \le u_1$ *and* $1 \le j \le n_A$, *an* $\mathrm{MCD}(D_1, D_2)$ *with* $D_1 = \mathrm{OA}(s^u, u_1, s, u_1)$, $D_2 = \mathrm{LHD}(s^u, n_A)$ *can be obtained*, *or*,
(ii) *choose* $\mathbf{z}_i \in \mathcal{A}$ *and* $\mathbf{x}_j = \mathbf{e}_j$ *for* $1 \le i \le n_A$ *and* $1 \le j \le u_1$, *an* $\mathrm{MCD}(D_1, D_2)$ *with* $D_1 = \mathrm{OA}(s^u, n_A, s, 2)$, $D_2 = \mathrm{LHD}(s^u, u_1)$ *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 $u_1 \le u$ 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. [7] by choosing some linear combinations of $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$ 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 $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$ 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* $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$ *defined above*, *let* $\mathbf{z} = \sum_{i=1}^{u_1} \lambda_i \mathbf{e}_i$ *with at least two nonzero coefficients*, *where* $\lambda_i \in \mathrm{GF}(s)$. *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 $\{\alpha \mathbf{e}_i \mid \alpha \in \mathrm{GF}(s) \setminus \{0\}, i = 1, \ldots, u_1\}$, 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 $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$ for D_1, we use a subset $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} \subset \mathcal{A}$ to construct $(u-1)$-dimensional subspaces $\{O(\mathbf{x}_1), \ldots, O(\mathbf{x}_k)\}$, where $k < n_A$. Next, the section discusses an approach to find such a subset.

3.2. Subspace construction

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

One building block of the proposed approach is some disjoint groups of $\mathcal{A}$. To partition $\mathcal{A}$ into different groups, note that for $1 \le j \le u_1$, 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,

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

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

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

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* $1 \le v \le n_B$, *any* $\mathbf{z} \in \bigcap_{i=1}^{v} \overline{E}_i$ *and any* $\mathbf{x} \in \bigcup_{i=1}^{v} \mathcal{A}_i$, *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 $\bigcap_{i=1}^{v} \overline{E}_i$, and $\mathbf{x}_j$ from $\bigcup_{i=1}^{v} \mathcal{A}_i$, that is exactly the method Theorem 2 adopts.

So far, it remains to resolve the question that what the elements are in $\bigcap_{i=1}^{v} \overline{E}_i$ for $1 \le v \le n_B$. The answer is not difficult for $v = 1$, and that for $v = n_B$ can be found in Proposition 6 in the Appendix for interested readers. For $1 < v < n_B$, the explicit form for elements in $\bigcap_{i=1}^{v} \overline{E}_i$ depends on the specific sets $\overline{E}_1, \dots, \overline{E}_v$. Thus, we cannot express the elements in $\bigcap_{i=1}^{v} \overline{E}_i$ using a general form. However, we are able to compute the number of elements in $\bigcap_{i=1}^{v} \overline{E}_i$ 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, $|\bigcap_{i=1}^{v} \overline{E}_i|$, 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* $n^* \le n_B$. *We have that for* $1 \le v \le n^*$ *and* $1 \le i_1 < i_2 < \cdots < i_v \le n_B$, *the set* $\bigcap_{j=1}^{v} \overline{E}_{i_j}$ *contains* $f(v)$ *elements with*

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

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

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.

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

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

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	2
0	1	1	0	0	1	2	1	2	0	2	2	0	0	2	1	2	1
1	0	1	0	1	0	2	2	1	2	0	2	0	2	0	1	1	2
0	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	2
0	1	1	0	0	1	1	2	2	0	2	2	0	0	2	2	1	1
1	0	2	0	2	0	1	2	1	2	0	1	0	1	0	2	1	2
0	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	2
0	1	1	0	0	2	1	2	1	0	2	2	0	0	1	2	1	2
1	0	2	0	1	0	1	2	2	2	0	1	0	2	0	2	1	1
0	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	2
0	1	1	0	0	2	1	1	2	0	2	2	0	0	1	2	2	1
1	0	1	0	2	0	1	2	1	2	0	2	0	1	0	2	1	2
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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.

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 $1 \le v \le n^*$, obtain $\bigcap_{j=1}^{v} \overline{E}_{i_j}$ which has $f(v)$ elements as shown in Proposition 2. Define E_v^* to be the subset of $\bigcap_{j=1}^{v} \overline{E}_{i_j}$ 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 $\mathcal{A}_v^* = \bigcup_{j=1}^{v} \mathcal{A}_{i_j}$.

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 $D_1 = \mathrm{OA}(s^u, g(v), s, 2)$, $D_2 = \mathrm{LHD}(s^u, vs^{u-u_1})$ 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 $D_1 = \mathrm{OA}(s^u, vs^{u-u_1}, s, 2)$, $D_2 = \mathrm{LHD}(s^u, g(v))$ 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 $\bigcap_{j=1}^{3} \overline{E}_j$ and $\bigcup_{j=1}^{3} \mathcal{A}_j$. In Step 1, $f(3) = 8$, hence $g(3) = 4$. The four elements in $\bigcap_{j=1}^{3} \overline{E}_j$ 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 $\bigcup_{j=1}^{3} \mathcal{A}_j = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_9\}$ 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

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

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

further let $\tilde{D}_2 = (\mathbf{d}_1, \ldots, \mathbf{d}_9)$, 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 ◇.

3.3. The maximum value of n^*

Both Proposition 2 and Theorem 2 require a set of vectors $\{\mathbf{b}_{i_1}, \ldots, \mathbf{b}_{i_{n^*}}\}$ 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 $\mathbf{b}_1 = (1, \ldots, 1, 0, \ldots, 0)$, $\mathcal{A} = \mathcal{A}_1 = \{(1, \ldots, 1, x_{u_1+1}, \ldots, x_u) \mid x_i \in \{0, 1\}\}$, and $\overline{E}_1$ contains all the combinations of $\lambda_1 \mathbf{e}_1 + \cdots + \lambda_{u_1} \mathbf{e}_{u_1}$ that are not orthogonal to column vectors of $\mathcal{A}_1$. Note that $\overline{E}_1$ consists of all combinations with odd numbers of $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$. 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 $\mathcal{A} = \mathcal{A}_1$, $\overline{E}_1 = \{\alpha \mathbf{e}_1 \mid \alpha \in \mathrm{GF}(s) \setminus \{0\}\}$, $v = 1$, $f(1) = s - 1$, $g(1) = 1$ 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 $s - 1$ choices as $(1, \alpha_1)^T, (1, \alpha_2)^T, \ldots, (1, \alpha_{s-1})^T$ for $\alpha_i \in \mathrm{GF}(s)$, hence $\mathbf{b}_i = (1, \alpha_i, 0, \ldots, 0)^T$. As any two vectors of $\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_{s-1}\}$ 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 [1]. 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 $\{\mathbf{b}_1, \ldots, \mathbf{b}_{n^*}\}$ are independent. We have*

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

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$(s^u, s - v + 1)$

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 $\mathrm{OA}(s^{u_1}, m, s, u_1)$. It shall be noted that, however, it is possible to give an upper bound tighter than that given by Proposition 3, for example, for $u_1 = 2$, the maximum value of n^* is $s - 1$, but the maximum value of m in an $\mathrm{OA}(s^2, m, s, 2)$ 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 $\overline{u}_1 = u - u_1$, 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 jth column is determined by the (i, j)th entry $B_{u_1}(i, j)$ as follows:

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

Hence the jth column is labeled by bold $\mathbf{j - 1}$ 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

Table 5. $\mathrm{MCD}(D_1, D_2)$s with 3^u runs by Theorem 1, $u = 2, 3, 4, 5$

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

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

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

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

B_2

0	**1**
1	1
1	2

B_3

0	**1**	**2**	**3**
1	1	1	1
1	1	2	2
1	2	1	2

B_4

0	**1**	**2**	**3**	**4**	**5**	**6**	**7**
1	1	1	1	1	1	1	1
1	1	1	1	2	2	2	2
1	1	2	2	1	1	2	2
1	2	1	2	1	2	1	2

B_5

0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
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

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 $\{\mathbf{b}_{i_1}, \ldots, \mathbf{b}_{i_{n^*}}\}$ required by Theorem 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, Draguljić, Santner and Dean [3], Joseph, Gul and Ba [11], and Sun and Tang [18]. 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 [12]; 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 $\overline{v}_1 = v_2$ and $\overline{v}_2 = v_1$.

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

For practical application, given parameters $1 \le u_1, u_1' \le u$, item (ii) of Theorem 2 can construct an MCD(D_1, D_2) with $D_1 = \mathrm{OA}(2^u, 2^{u-u_1}, 2, 3)$ and $D_2 = \mathrm{LHD}(2^u, 2^{u_1-1})$, and item (i) can construct an MCD(D_1, D_2) with $D_1 = \mathrm{OA}(2^u, 2^{u_1'-1}, 2, 3)$ and $D_2 = \mathrm{LHD}(2^u, 2^{u-u_1'})$. 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

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

where $\mathbf{y}_i \ne \mathbf{y}_j$ for $i \ne j$. 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 $1 \le i \le 2^{u-u_1}$, define $\eta_i = (\mathbf{x}_0^T, \overline{\mathbf{y}}_i^T)^T$, where $\overline{\mathbf{y}}_i$ is the anti-mirror vector of $\mathbf{y}_i$. We have $\eta_i \in O(\mathbf{x}_i)$ as $\eta_i^T\mathbf{x}_i = \mathbf{x}_0^T\mathbf{1}_{u_1} + \overline{\mathbf{y}}_i^T\mathbf{y}_i = 0$ 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 η_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* $2 \le u_1 < u - 1$, *the design* $\tilde{D}_2$ *obtained by the anti-mirror arrangement is an* $\mathrm{OA}(2^u, 2^{u-u_1}, 2^{u-1}, 1)$ *achieving stratifications on a* $2 \times 2 \times 2$ *grid of any three dimensions.*

For $s \ge 2$, 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* $k \le (s^{u-1} - 1)/(s - 1)$, *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. [7] for two-level qualitative factors to any s-level qualitative factors. The *Construction 2* of He, Lin and Sun [6] 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 $\mathrm{OA}(s^{u-1}, (s^{u-1}-1)/(s-1), s, 2)$. 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 $1 \le i \le s$, 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 respectively 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 $2 \le i \le s$, 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 $1 \le k < s+1$, and choosing $\mathbf{z}_1, \dots, \mathbf{z}_m$ from the set of $\bigcup_{j=k+1}^{s+1} O(\mathbf{x}_j) \setminus (\bigcup_{i=1}^{k} O(\mathbf{x}_i))$, one can obtain the marginally coupled design provided by *Construction 2* of He, Lin and Sun [6].

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

Proof of Theorem 1. 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), $O(\mathbf{x}_i) \ne O(\mathbf{x}_j)$ when $i \ne j$, $\mathbf{d}_i$ cannot be transformed to $\mathbf{d}_j$ by level permutations. Thus D_2's are non-cascading Latin hypercubes. □

Proof of Proposition 1. Suppose $\mathbf{z} = \sum_{i=1}^{u_1} \lambda_i \mathbf{e}_i$ has l nonzero coefficients $\lambda_{i_1}, \dots, \lambda_{i_l}$, where $1 \le i_j \le u_1$ and $2 \le l \le u_1$. Denote by $\lambda^* = \sum_{j=1}^{l-1} \lambda_{i_j}$, and let $\mathbf{x} = (x_1, \dots, x_u)^T$. If λ^* 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 $l - 1 \ge 2$, 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 $\alpha_2 \ne 1$, hence $x_{i_l} \ne 0$ 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 $\mathbf{z} \in O(\mathbf{x})$. □

Proof of Proposition 2. 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

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

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

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

For $u_1 + 1 \le v \le n^*$, the intersection of any $t \ge u_1$ 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

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

□

Proof of Theorem 2. Followed by Lemma 4, for any $\mathbf{z} \in \bigcap_{j=1}^{v} \overline{E}_{i_j}$ and $\mathbf{x} \in \bigcup_{j=1}^{v} \mathcal{A}_{i_j}$, 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. Since any u_1 vectors of $\{\mathbf{b}_1, \ldots, \mathbf{b}_{n^*}\}$ are independent, one can use them to obtain an $\mathrm{OA}(s^{u_1}, n^*, s, u_1)$. 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 $\mathrm{OA}(s^{u_1}, m, s, u_1)$ 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 [8]. □

Proof of Proposition 4. It is straightforward to see $\tilde{D}_2$ is an $\mathrm{OA}(2^u, 2^{u-u_1}, 2^{u-1}, 1)$. 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 $1 \le p < q < l \le 2^{u-u_1}$. Let $\mathbf{c}_i = \lfloor \mathbf{d}_i / 2^{u-2} \rfloor$. As $\mathbf{d}_i = A_i \cdot (2^{u-2}, \ldots, 2, 1)^T$, $\mathbf{c}_i$ 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 η_i. As $\mathbf{y}_i \neq \mathbf{y}_j$ for $i \neq j$, we have $\overline{\mathbf{y}}_i \neq \overline{\mathbf{y}}_j$. Since the last $u - u_1$ entries of η_i is $\overline{\mathbf{y}}_i$, η_p, η_q and η_l are three different columns. In addition, $\eta_p + \eta_q \neq \eta_l$ because the first u_1 entries of η_p, η_q, η_l are equal to $\mathbf{x}_0 = (1, 1, 0, \ldots, 0)^T$. As a result, η_p, η_q, η_l are three independent column vectors. Thus, the array $(\mathbf{c}_p, \mathbf{c}_q, \mathbf{c}_l)$ is an $\mathrm{OA}(2^u, 3, 2, 3)$, and the conclusion follows. □

Proof of Proposition 5. In the subspace construction of Theorem 2, for $i = 1, \ldots, k$, 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 $k \le (s^{u-1} - 1)/(s - 1)$, one can always choose $\mathbf{y}_i \in O(\mathbf{x}_i)$, such that $\mathbf{y}_i \neq \alpha \mathbf{y}_j$ for $1 \le i \neq j \le k$ and any $\alpha \in \mathrm{GF}(s)$. 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 $\{A_1, \ldots, A_k\}$, the first k columns form an $\mathrm{OA}(s^u, k, s, 2)$, which guarantees $\tilde{D}_2$ to achieve stratifications on an $s \times s$ grid of any two dimensions. □

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

Proof. For $s = 2$, we have $n_B = 1$, $\mathcal{A} = \mathcal{A}_1$, and $\mathbf{b}_1 = (1, \ldots, 1, 0, \ldots, 0)^T$ 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 $\mathbf{z} \in \bigcap_{i=1}^{n_B} \overline{E}_i$, $\mathbf{z} \notin O(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{A}$ by Lemma 4. Therefore, for $s > 2$, the possible elements in $\bigcap_{i=1}^{n_B} \overline{E}_i$ can only be $\mathbf{z} = \alpha \mathbf{e}_j$ for any $\alpha \in \mathrm{GF}(s) \setminus \{0\}$ and $j = 1, \ldots, u_1$, according to Proposition 1, while $\mathbf{e}_j \in \bigcap_{i=1}^{n_B} \overline{E}_i$, for $j = 1, \ldots, u_1$. Combining these two results, item (ii) follows. □

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