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On the maximin distance properties of orthogonal designs via the rotation

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Abstract Space-filling designs are widely used in computer experiments. They are frequently evaluated by the orthogonality and distance-related criteria. Rotating orthogonal arrays is an appealing approach to constructing orthogonal space-filling designs. An important issue that has been rarely addressed in the literature is the design selection for the initial orthogonal arrays. This paper studies the maximin L_2-distance properties of orthogonal designs generated by rotating two-level orthogonal arrays under three criteria. We provide theoretical justifications for the rotation method from a maximin distance perspective and further propose to select initial orthogonal arrays by the minimum G_2-aberration criterion. New infinite families of orthogonal or 3-orthogonal U-type designs, which also perform well under the maximin distance criterion, are obtained and tabulated. Examples are presented to show the effectiveness of the constructed designs for building statistical surrogate models.

Keywords computer experiment, Latin hypercube design, minimum G_2-aberration, space-filling design, U-type design

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1 Introduction

Computer experiments are being increasingly applied in scientific and industrial research [6, 18]. One of the primary goals of a computer experiment is to build a rapidly computable surrogate model to approximate an expensive-to-run computer simulation code. The performance of a surrogate model relies heavily on the space-filling properties of the experimental design. Latin hypercube designs (LHDs) are widely used in computer experiments due to their maximum projection property for investigating each factor [12]. U-type designs, which allow flexibility in the number of levels, have also been proposed as extensions of LHDs in computer or physical experiments [2]. To improve the space-filling properties of an LHD or a U-type design, many different types of space-filling measures have been proposed (see, for examples, [9, 12, 13, 17, 34]).

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Among various space-filling criteria, the maximin distance [8] and orthogonality [15] are two of the most widely used during the last few decades. The maximin distance criterion aims to maximize the minimum distance between any two runs of a design. Some advances on this topic can be found in [1, 25, 29, 33]. The orthogonality criterion optimizes designs by minimizing the correlations among factors. It can be viewed as a useful stepping stone to space-filling designs [2]. There are fruitful construction methods for orthogonal designs [12]. Among them, Steinberg and Lin [20] were the first to propose constructing orthogonal LHDs by rotating groups of factors of orthogonal arrays. This method, which we call the rotation method, is simple and exhibits great theoretical beauty. In recent years renewed interest have been seen in this method (see, e.g., [11, 16, 23] for developments on orthogonal LHDs and [22, 24] for generalizations to orthogonal U-type designs).

The two criteria, the orthogonality and maximin distance, have some connections [26, 27]; however, they may not agree with each other in all the circumstances. In a pioneering work, Joseph and Hung [10] proposed orthogonal-maximin LHDs which simultaneously optimize the two criteria. Such designs are ideal for computer experiments. A statistical justification is given under the Gaussian process modeling (also known as kriging). Suppose that the real function of the computer simulation code is $y(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, \ldots, x_m)$. It is common to fit a universal kriging model with linear trends

$$Y(\boldsymbol{x}) = \beta_0 + \sum_{k=1}^{m} \beta_k x_k + Z(\boldsymbol{x}) \tag{1.1}$$

as the surrogate model to approximate $y(\boldsymbol{x})$, where $\beta_0, \ldots, \beta_m$ are some unknown constants, $Z(\boldsymbol{x})$ is a stationary Gaussian process with the mean 0 and covariance function $\sigma^2 R(\cdot)$. A popular choice for the correlation function $R(\cdot)$ is the exponential, i.e.,

$$R(\boldsymbol{x}_i - \boldsymbol{x}_j; \theta) = \exp\bigg(-\theta \sum_{k=1}^{m} |x_{ik} - x_{jk}|^p\bigg), \quad \theta \in (0, \infty), \quad p \in (0, 2].$$

When $p = 2$, $R(\cdot)$ is called the Gaussian correlation function. The maximum entropy criterion is to find a design that maximizes the determinant of the variance-covariance matrix of the responses [10, 19]. Joseph and Hung [10] showed that orthogonal-maximin designs are asymptotically optimal under the maximum entropy criterion as $\theta \to \infty$. Thus, orthogonal-maximin designs are expected to perform well under the kriging model (1.1).

Although orthogonal-maximin designs are appealing, their construction is challenging. The existing algorithm construction in [10] can be computationally inefficient when the target design is large. There is no guarantee that the resulting designs will truly be orthogonal and maximin. Hence, it is crucial to develop efficient algebraic constructions. This paper aims to investigate whether the rotation method can generate designs with both orthogonality and good distance properties. The designs generated by rotating orthogonal arrays are naturally orthogonal. However, observations have indicated that the choice of the initial orthogonal array can substantially affect the final design's space-filling properties (see Section 3 and later examples). Therefore, the orthogonal arrays in the rotation method need to be carefully selected. To address this issue, we show some properties of orthogonal designs generated by rotating two-level orthogonal arrays under three maximin distance measures. Based on these theoretical results, we propose to use the minimum G_2-aberration criterion [5] to select initial orthogonal arrays in the rotation method. As a result, new infinite families of orthogonal or 3-orthogonal U-type designs, which also perform well under the maximin distance criterion, are obtained and tabulated.

The main contribution of this work is threefold. First, the original rotation method proposed by [23] is for LHDs. We generalize it to U-type designs incorporating LHDs as a special case. Second, the existing literature on the rotation method focuses on orthogonal designs only [16, 20, 22, 23]. This paper studies the properties of such orthogonal designs under the maximin distance criteria for the first time. We show that the rotation of two-level orthogonal arrays yields orthogonal U-type designs with the best inter-site L_2-distance variance among all the U-type designs of the same size. This provides a new justification for the rotation method from a maximin distance viewpoint. We also establish explicit connections between the final design's distance measures and the initial orthogonal array's properties for the rotation method. Third, we propose a new construction method for space-filling designs by rotating minimum G_2-aberration orthogonal arrays and show its maximin distance optimality. The obtained designs outperform existing designs under both the orthogonality and maximin criteria. They are also expected to perform well in building Gaussian process models with linear trends in computer experiments.

The rest of this paper is organized as follows. In Section 2, we introduce some notation and background. In Section 3, we provide motivating examples that compare the distance properties of several orthogonal LHDs by the rotation method. In Section 4, we present the main results. We first generalize the rotation method in [23] to orthogonal U-type designs, then obtain several theoretical properties of the rotation method under three distance-related criteria, and finally construct several new families of orthogonal-maximin designs by rotating minimum G_2-aberration orthogonal arrays. In Section 5, we provide an application to demonstrate the effectiveness of our designs in building statistical surrogate models. In Section 6, we conclude the paper with some discussions. All the proofs are deferred to Appendix A.

2 Notation and maximin distance measures

An s-level design with n runs and m factors, denoted by (n, s^m), is represented by an $n \times m$ matrix taking values from s equally spaced numbers. Without loss of generality, suppose that the s levels are

$$\{j - (s-1)/2 \mid j = 0, \ldots, s-1\}$$

such that their mean is zero. An (n, s^m) design D is called a U-type design if each of the s levels appears equally often in each column. In particular, a Latin hypercube design is a U-type design with $s = n$ and is denoted by LHD(n, m). A two-level orthogonal array of strength $t \geqslant 2$ and index λ, denoted by OA$(n, m, 2, t)$, is a U-type $(n, 2^m)$ design such that in each of its $n \times t$ subarrays every possible t-tuple occurs exactly $\lambda = n/2^t$ times. It is noteworthy that the two levels of an OA$(n, m, 2, t)$ are $\pm 1/2$ in this paper, instead of ± 1 or $\{0, 1\}$ as per convention.

Let $D = (x_{ik})$ be a U-type (n, s^m) design and ρ_{jk} be the sample correlation between the j-th and k-th columns in D. By [15], the mean squared correlation of D is defined as

$$\rho^2(D) = \binom{m}{2}^{-1} \sum_{j=1}^{m-1} \sum_{k=j+1}^{m} \rho_{jk}^2.$$

A design D is called orthogonal if $\rho^2(D) = 0$. If D is orthogonal and satisfies the constraint that the sum of elementwise products of any three columns (no matter whether they are distinct or not) is zero, then D is called 3-orthogonal. Orthogonality or 3-orthogonality is the favourable property for computer experimental designs [12].

The L_2-distance between the i-th row $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{im})$ and the j-th row $\boldsymbol{x}_j = (x_{j1}, \ldots, x_{jm})$ in D is defined as $d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{k=1}^{m} (x_{ik} - x_{jk})^2$. Here, the squared Euclidean distance is adopted to ensure that $d(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is an integer and is additive, i.e.,

$$d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{k=1}^{m} d(x_{ik}, x_{ik}).$$

We consider three distance-based criteria, all aiming at optimizing $\{d(\boldsymbol{x}_i, \boldsymbol{x}_j) \mid \boldsymbol{x}_i, \boldsymbol{x}_j \in D, 1 \leqslant i < j \leqslant n\}$, i.e., the set of all $\binom{n}{2}$ inter-site distances in D. The first one is employed to maximize

$$d(D) = \min\{d(\boldsymbol{x}_i, \boldsymbol{x}_j) \mid \boldsymbol{x}_i, \boldsymbol{x}_j \in D, 1 \leqslant i < j \leqslant n\},$$

which is the original maximin distance criterion proposed by [8]. For a U-type (n, s^m) design, it is easy to verify that the average of all the $\binom{n}{2}$ distances is

$$\bar{d} = \binom{n}{2}^{-1} \sum_{1 \leqslant i < j \leqslant n} d(\boldsymbol{x}_i, \boldsymbol{x}_j) = nm(s^2 - 1)/(6n - 6), \tag{2.1}$$

which implies a useful upper bound of the minimum distance [35].

Lemma 2.1. *For a U-type (n, s^m) design $D = (x_{ij})$,*

$$d(D) \leqslant \lfloor \bar{d} \rfloor = \lfloor nm(s^2-1)/(6n-6) \rfloor,$$

where $\lfloor x \rfloor$ denotes the largest integer not exceeding x.

In particular, for LHD(n, m) the upper bound becomes $\lfloor n(n+1)m/6 \rfloor$. Based on Lemma 2.1, we define $d_{\text{eff}}(D) = d(D)/\lfloor \bar{d} \rfloor$ as the distance efficiency for evaluating a U-type design D.

The minimum distance is a the-larger-the-better metric. We also consider two the-smaller-the-better criteria. One is used to minimize

$$\phi_q(D) = \binom{n}{2}^{-1} \sum_{1 \leqslant i < j \leqslant n} q^{d(\boldsymbol{x}_i, \boldsymbol{x}_j)}, \quad q \in (0,1).$$

This metric was used in [34] and can be viewed as an extension of the maximin distance criterion. The other is used to minimize the distance variance, or equivalently,

$$V(D) = \sum_{1 \leqslant i < j \leqslant n} (d(\boldsymbol{x}_i, \boldsymbol{x}_j) - \bar{d})^2.$$

Minimizing $V(D)$ is a natural criterion which is originated from the fact that a maximin distance design tends to optimize the second moment of all the pairwise distances. This metric has also been justified by [26, 29].

3 Motivating examples

This section presents two motivating examples in which the maximin distance properties of several orthogonal LHDs are compared.

Example 3.1. Steinberg and Lin [20] constructed an orthogonal LHD$(16, 12)$. Denote this design by E (see Table 1). Its original levels are divided by two in order to adapt our setting. Let E_1, E_2, E_3 and E_4 be four 16×8 subdesigns selecting columns indexed by $\{2, 3, 4, 6, 7, 8, 10, 12\}$, $\{1, 2, 3, 4, 5, 6, 7, 8\}$, $\{1, 2, 3, 4, 9, 10, 11, 12\}$ and $\{5, 6, 7, 8, 9, 10, 11, 12\}$ from E, respectively. Let E_5 be the orthogonal LHD$(16, 8)$ in [20, Example 2] with the original levels divided by two. The design E_5 shares the same first 4 columns as E, and its last 4 columns are shown in Table 1. All of the E_i $(i = 1, \ldots, 5)$ are orthogonal LHD$(16, 8)$s, but have different space-filling properties. Table 2 compares the distance variances, ϕ_q values $(q = 0.99)$, minimum L_2-distances and the corresponding distance efficiencies of the five designs. Designs E_2, E_3, E_4 and E_5 have the same distance variance and are better than E_1. Designs E_2 and E_3 have the same ϕ_q value. Design D_5 is the best under all the criteria; furthermore, it is also 3-orthogonal. All of these observations can be explained theoretically by Theorems 4.3 and 4.5 and (ii) and (iii) of Corollary 4.11.

Example 3.2. Let E^* be the LHD$(16, 12)$ given in Table 3. This design is new, and one can check that it is orthogonal. In fact, it is also an orthogonal LHD constructed by the rotation method (see Example 4.9). Compared with Steinberg and Lin's LHD E in Table 1, E^* is more space-filling under the maximin distance criterion. We have

$$\begin{aligned} &V(E) = V(E^*) = 5.595 \times 10^5, \\ &\phi_q(E) = 5.322 \times 10^{-3} > \phi_q(E^*) = 4.969 \times 10^{-3} \ (q = 0.99), \\ &d(E) = 425 < d(E^*) = 510 \end{aligned}$$

and

$$d_{\text{eff}}(E) = 0.781 < d_{\text{eff}}(E^*) = 0.938.$$

Table 1 Steinberg and Lin's orthogonal LHD(16, 12) E (left) and orthogonal LHD(16, 8) E_5 (right, only the last 4 columns are presented, and the first 4 columns are the same as E), where the levels have been multiplied by two

1	2	3	4	5	6	7	8	9	10	11	12
−15	5	9	−3	7	11	−11	7	−9	3	−15	5
−13	1	1	13	−7	−11	11	−7	−1	−13	−13	1
−11	7	−7	−11	13	−1	−1	−13	9	−3	15	−5
−9	3	−15	5	−13	1	1	13	1	13	13	−1
−7	−11	11	−7	11	−7	7	11	5	15	−3	−9
−5	−15	3	9	−11	7	−7	−11	13	−1	−1	−13
−3	−9	−5	−15	1	13	13	−1	−5	−15	3	9
−1	−13	−13	1	−1	−13	−13	1	−13	1	1	13
1	13	13	−1	−9	3	−15	5	11	−7	7	11
3	9	5	15	9	−3	15	−5	3	9	5	15
5	15	−3	−9	−3	−9	−5	−15	−11	7	−7	−11
7	11	−11	7	3	9	5	15	−3	−9	−5	−15
9	−3	15	−5	−5	−15	3	9	−7	−11	11	−7
11	−7	7	11	5	15	−3	−9	−15	5	9	−3
13	−1	−1	−13	−15	5	9	−3	7	11	−11	7
15	−5	−9	3	15	−5	−9	3	15	−5	−9	3

5	6	7	8
−15	5	9	−3
−1	−13	−13	1
7	11	−11	7
9	−3	15	−5
11	−7	7	11
5	15	−3	−9
−3	−9	−5	−15
−13	1	1	13
13	−1	−1	−13
3	9	5	15
−5	−15	3	9
−11	7	−7	−11
−9	3	−15	5
−7	−11	11	−7
1	13	13	−1
15	−5	−9	3

Table 2 Comparison of five orthogonal LHD(16, 8)s

Design	E_1	E_2	E_3	E_4	E_5
$10^{-5}V(E_i)$	15.168	8.704	8.704	8.704	8.704
$10^2\phi_q(E_i)$	5.264	3.927	3.927	3.601	3.069
$d(E_i)$	76.000	170.000	170.000	255.000	340.000
$d_{\text{eff}}(E_i)$	0.210	0.470	0.470	0.704	0.939

Table 3 A new orthogonal LHD(16, 12) E^*, where the levels have been multiplied by two

1	2	3	4	5	6	7	8	9	10	11	12
−15	−5	−9	−3	−15	−5	−9	−3	−15	−5	−9	−3
−13	−1	−1	13	9	3	−15	−5	7	−11	11	7
−11	−7	7	−11	3	−9	−5	15	13	1	1	−13
−9	−3	15	5	−5	15	−3	9	−5	15	−3	9
−7	11	−11	−7	−3	9	5	−15	−1	13	13	1
−5	15	−3	9	5	−15	3	−9	9	3	−15	−5
−3	9	5	−15	15	5	9	3	3	−9	−5	15
−1	13	13	1	−9	−3	15	5	−11	−7	7	−11
1	−13	−13	−1	−1	13	13	1	5	−15	3	−9
3	−9	−5	15	7	−11	11	7	−13	−1	−1	13
5	−15	3	−9	13	1	1	−13	−7	11	−11	−7
7	−11	11	7	−11	−7	7	−11	15	5	9	3
9	3	−15	−5	−13	−1	−1	13	11	7	−7	11
11	7	−7	11	11	7	−7	11	−3	9	5	−15
13	1	1	−13	1	−13	−13	−1	−9	−3	15	5
15	5	9	3	−7	11	−11	−7	1	−13	−13	−1

4 Main results

This section shows the main results of the maximin distance properties of the orthogonal designs via the rotation. To the best of our knowledge, Sun and Tang's method in [23] is the most powerful rotation method, and it includes several previous methods as special cases. Thus, we focus on the method in [23] for rotating two-level orthogonal arrays. Their original construction is for orthogonal LHDs. First, we generalize it in order to make it adaptable for orthogonal U-type designs in Subsection 4.1.

4.1 The method of rotating orthogonal arrays

An $m\times m$ matrix R is called a rotation matrix of order m if $R^{\mathrm{T}}R$ is proportional to the identity matrix I_m. Generally, the rotation method first selects an $n \times m$ fractional factorial design, D, and then rotates its factors by R to produce a new design $E = DR$.

For $u, v = 2, 3, \dots$, recursively define

$$R_{10} = \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}, \quad R_{u0} = \begin{pmatrix} 2^{2^{(u-1)}} & -1 \\ 1 & 2^{2^{(u-1)}} \end{pmatrix} \otimes R_{(u-1)0},$$

$$Q_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Q_u = Q_1 \otimes Q_{u-1}$$

and

$$R_{u1} = \begin{pmatrix} 2R_{u0} & -Q_u \\ Q_u & 2R_{u0} \end{pmatrix}, \quad R_{uv} = \begin{pmatrix} 2R_{u(v-1)} & -Q_{u+v-1} \\ Q_{u+v-1} & 2R_{u(v-1)} \end{pmatrix},$$

where $\otimes$ is the Kronecker product. Then R_{uv} is a rotation matrix of order 2^{u+v} for $u \geqslant 1$ and $v \geqslant 0$.

Lemma 4.1. *Suppose that $D = (D_1, \dots, D_k)$ is an $\mathrm{OA}(\lambda 2^{2^u}, k2^u, 2, t)$ with $t \geqslant 2$ and $u \geqslant 1$ such that each D_j is a full factorial of 2^u factors and index λ. An orthogonal U-type (n, s^m) design with $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ and $m = k2^{u+v}$ $(v \geqslant 0)$ can be constructed by using the rotation matrix R_{uv}. Furthermore, if $t \geqslant 3$, the constructed design is 3-orthogonal.*

The proofs of Lemma 4.1 and later results are provided in Appendix A. When $\lambda = 1$, Lemma 4.1 yields orthogonal LHDs, which corresponds to the two-level case of [23, Theorem 1].

The construction details for the orthogonal designs in Lemma 4.1 are now described. If $v = 0$, letting $R = I_k \otimes R_{u0}$, we see that $E = DR$ is an orthogonal U-type (n, s^m) design with $n = \lambda 2^{2^u}$, $s = 2^{2^u}$ and $m = k2^u$. Specifically, the case of $\lambda = 1$ is exactly the rotation method in [20]. If $v \geqslant 1$, the construction includes two steps. First, enlarge D iteratively to obtain an $\mathrm{OA}(n, m, 2, t)$, denoted by D^v, with $n = \lambda 2^{2^u+v}$ and $m = k2^{u+v}$, by doubling each D_j v times, i.e.,

$$D^v = (D_1^v, \dots, D_k^v) \quad \text{and} \quad D_j^v = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes D_j^{(v-1)}, \tag{4.1}$$

where D_i^0 denotes D_i. Then rotate D^v by R to obtain an orthogonal U-type (n, s^m) design, as desired in Lemma 4.1, where $R = I_k \otimes R_{uv}$.

4.2 Distance variance optimality

This and the next two subsections are devoted to investigating the properties of orthogonal designs via Lemma 4.1 under the distance variance, $\phi_q(D)$ and $d(D)$ criteria, respectively. We start by establishing a novel decomposition and a lower bound of distance variance for a general U-type design.

Theorem 4.2. *For a U-type (n, s^m) design $D = (x_{ij})$,*

$$V(D) = 72^{-1} n^2 m(m-1)(s^2-1)^2 \rho^2(D) + n \sum_{i=1}^{n} d^2(\boldsymbol{x}_i, 0) - C(n, m, s), \tag{4.2}$$

where $d(\boldsymbol{x}_i, 0) = \sum_{k=1}^{m} x_{ik}^2$ *and*

$$C(n,m,s) = [144(n-1)]^{-1} n^2 m[(m-2)n + m + 2](s^2-1)^2.$$

Furthermore,

$$V(D) \geqslant [72(n-1)]^{-1} n^2 m(n-m-1)(s^2-1)^2 \tag{4.3}$$

with the equality holding if and only if D *is orthogonal and any row is* L_2*-equidistant from the origin.*

By the rotation method, the constructed orthogonal U-type (n, s^m) design in Lemma 4.1 is $E = D^v R$, where D^v is an $\mathrm{OA}(n, m, 2, t)$ defined in (4.1) and $R = I_k \otimes R_{uv}$. Clearly, any row $\boldsymbol{x}$ in D^v has $d(\boldsymbol{x}, 0) = m/4$. Because the rotation is isometric, all the rows in E are also equidistant from the origin. Hence, by Theorem 4.2, the following statement holds.

Theorem 4.3. *Let* E *be an orthogonal U-type* (n, s^m) *design with* $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ *and* $m = k2^{u+v}$ $(v \geqslant 1)$ *constructed by the rotation method in Lemma* 4.1*. Then* E *has the minimum* L_2*-distance variance and achieves the lower bound in* (4.3) *among all the U-type* (n, s^m) *designs.*

Theorem 4.3 indicates that all the designs generated by rotating two-level orthogonal arrays are optimal under the distance variance criterion. It provides a new theoretical justification for the rotation method from a distance-based viewpoint.

Example 4.4 (Example 3.1 continued)**.** Let $D = (D_1, D_2, D_3)$ be the regular $\mathrm{OA}(16, 12, 2, 2)$ from [20]. Each D_i is a full 2^4 factorial, where D_1 has four independent columns a_1, a_2, a_3 and a_4, D_2 has interaction columns a_1a_2, a_1a_3, $a_1a_2a_3$ and a_1a_4 and D_3 has interaction columns a_2a_3, a_2a_4, $a_1a_2a_4$ and $a_2a_3a_4$. The design E in Example 3.1 (see Table 1) is actually constructed by $E = DR$, where $R = I_3 \otimes R_{20}$. The designs E_2, E_3 and E_4 are also rotations of orthogonal arrays, i.e., $E_2 = (D_1R_{20}, D_2R_{20})$, $E_3 = (D_1R_{20}, D_3R_{20})$ and $E_4 = (D_2R_{20}, D_3R_{20})$. Let D_4 consist of four three-factor interaction columns. The design E_5 in Table 1 is constructed by $E_5 = (D_1R_{20}, D_4R_{20})$. By Theorem 4.3 we know that each E_i $(i = 2, 3, 4, 5)$ is optimal with the minimum distance variance among all the $\mathrm{LHD}(16, 8)$s. The design E_1 is inferior to E_2, E_3, E_4 and E_5 under the distance variance criterion. Theorem 4.3 also indicates that E_1 cannot be constructed by rotating any two-level orthogonal array.

4.3 Maximin ϕ_q-optimality

Subsection 4.2 shows that any orthogonal design produced by rotating a two-level orthogonal array is optimal under the distance variance criterion. However, different initial orthogonal arrays of the same size can be selected. To further distinguish them, we turn to the ϕ_q criterion.

Theorem 4.5. *Suppose that* D *is an* $\mathrm{OA}(\lambda 2^{2^u}, k2^u, 2, t)$ *with* $t \geqslant 2$ *satisfying the condition in Lemma* 4.1*. Let* E *be the orthogonal U-type* (n, s^m) *design with* $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ *and* $m = k2^{u+v}$ $(v = 0, 1, 2, \ldots)$ *constructed using* D *by the rotation method. We have*

$$\phi_q(E) = (n-1)^{-1}[(2^{-v}n - 1)\phi_{\tilde{q}}(D) + n(1-2^{-v})(q)^{\alpha m/2}],$$

where $\tilde{q} = q^{2^v\alpha}$ *and* $\alpha = (s^2-1)/3$*.*

Theorem 4.5 implies that the initial orthogonal array D in the rotation method determines the $\phi_q(E)$ values of all the orthogonal designs constructed by D. To acquire the best orthogonal design E, we need to choose a D with the minimum $\phi_{\tilde{q}}(D)$ value.

Let D be an $(n, 2^m)$-design and the corresponding full analysis of variance (ANOVA) model be

$$Y = X_0\boldsymbol{\alpha}_0 + X_1\boldsymbol{\alpha}_1 + \cdots + X_m\boldsymbol{\alpha}_m + \boldsymbol{\epsilon},$$

where Y is the vector of n responses, $\boldsymbol{\alpha}_0$ is the intercept, X_0 is an $n\times 1$ vector of 1's, $\boldsymbol{\alpha}_j$ is the vector of all the j-factor interactions, X_j is the $n \times \binom{m}{j}$ matrix given by the collection of products of j columns from $2D$ and $\boldsymbol{\epsilon}$ is the vector of random errors. Define $A_j(D) = n^{-2}X_0^{\mathrm{T}}X_jX_j^{\mathrm{T}}X_0$, $j = 0, \ldots, m$. It is obvious that $A_0(D) = 1$. The generalized wordlength pattern of D is the vector $(A_1(D), A_2(D), \ldots, A_m(D))$ (see [28]). The minimum G_2-aberration criterion sequentially minimizes $A_1(D), A_2(D), \ldots, A_m(D)$ (see [5]).

The next lemma is a result similar to [7, Theorem 1]. It follows from [34, Theorem 2] under the case of $s = 2$.

Lemma 4.6. *Let D be an $(n, 2^m)$ design. Then*

$$\phi_q(D) = (n-1)^{-1} n \left(\frac{1+q}{2}\right)^m \sum_{i=0}^{m} \left(\frac{1-q}{1+q}\right)^i A_i(D) - (n-1)^{-1}, \tag{4.4}$$

where $A_0(D) = 1$.

Lemma 4.6 shows that for two-level designs, ϕ_q can be linearly expressed by the generalized wordlength pattern. Because $[(1-q)/(1+q)]^i$ is positive and decreases geometrically with i, minimizing ϕ_q tends to agree with the minimum G_2-aberration criterion for two-level designs. Combining Theorem 4.5 with Lemma 4.6 shows that using minimum G_2-aberration orthogonal arrays in the rotation method tends to yield better orthogonal designs under the maximin criterion.

By choosing specific q values, we see that an exact equivalence can be established between the minimum G_2-aberration criterion and $\phi_q(D)$ in Lemma 4.6.

Corollary 4.7. *Let D be an $(n, 2^m)$ design. If*

$$n^2 M/(n^2 M + 2) \leqslant q < 1,$$

where

$$M = \binom{m}{\lfloor m/2 \rfloor},$$

then $\phi_q(D)$ is minimized if and only if D is a minimum G_2-aberration design.

Theorem 4.5 and Corollary 4.7 together imply that for given $v \geqslant 0$, there always exists a $\delta > 0$ such that for $1-\delta < q < 1$, minimizing ϕ_q of the orthogonal U-type (n, s^m) design with $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ and $m = k2^{u+v}$ is equivalent to finding a minimum G_2-aberration orthogonal array D for the rotation method.

Example 4.8 (Example 4.4 continued)**.** Let E_i $(i = 2, 3, 4, 5)$ be the orthogonal LHD(16, 8)s in Example 4.4. Designs (D_1, D_2) and (D_1, D_3) have the same generalized wordlength pattern $(0, 0, 5, 5, 2, 2, 1, 0)$. By Theorem 4.5 and Lemma 4.6, E_2 and E_3 have the same ϕ_q value. The generalized wordlength pattern of (D_2, D_3) is $(0, 0, 4, 5, 4, 2, 0, 0)$, and thus (D_2, D_3) is a better choice than (D_1, D_2) and (D_1, D_3) as initial orthogonal arrays for the rotation. The design (D_1, D_4) has the generalized wordlength pattern $(0, 0, 0, 14, 0, 0, 0, 1)$. It actually satisfies the condition in [3, Theorem 3], which means that it has minimum G_2-aberration. This explains why E_5 yields the smallest ϕ_q value in Table 2. Furthermore, (D_1, D_4) has strength three, and therefore the 3-orthogonality of E_5 follows from Lemma 4.1.

Using the rotation method in Lemma 4.1 for $v = 1$, we can also obtain four orthogonal LHD(32, 16)s, denoted by E_i^1 $(i = 2, 3, 4, 5)$ from the above OA(16, 8, 2, 2)s. By Theorem 4.5, the ϕ_q value of E_i^1 is determined by the generalized wordlength pattern of the initial OA(16, 8, 2, 2). Taking $q = 0.99$, we have $\phi_q(E_5^1) < \phi_q(E_4^1) < \phi_q(E_2^1) = \phi_q(E_3^1)$.

Example 4.9 (Example 3.2 continued)**.** The regular OA(16, 12, 2, 2) $D = (D_1, D_2, D_3)$ for generating E has the generalized wordlength pattern $(0, 0, 17, 38, 44, 52, 54, 33, 12, 4, 1, 0)$. Let D^* be the nonregular OA(16, 12, 2, 2) given in Table 4, which is actually constructed by using the method in [3, Theorem 3], up to some permutations of columns. It can be verified that the subdesigns indexed by columns 1–4, 5–8 and 9–12 of D^*, respectively, are all the full factorials. The LHD E^* is constructed by $E^* = D^* R$, where $R = I_3 \otimes R_{20}$. The generalized wordlength pattern of D^* is $(0, 0, 16, 39, 48, 48, 48, 39, 16, 0, 0, 1)$ and D^* has minimum G_2-aberration by [3, Theorem 3]. This justifies that $\phi_q(E^*) < \phi_q(E)$ in Example 3.2.

Using Lemma 4.1 for $v \geqslant 1$, we can further obtain two orthogonal LHD$(2^{v+4}, 3 \cdot 2^{v+2})$s from D and D^*. By Theorem 4.5, their ϕ_q values are completely determined by the generalized wordlength patterns of D and D^*, respectively.

Table 4 A nonregular OA(16, 12, 2, 2), where the levels have been multiplied by two

1	2	3	4	5	6	7	8	9	10	11	12
−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
−1	−1	−1	1	1	1	−1	−1	1	−1	1	1
−1	−1	1	−1	1	−1	−1	1	1	1	1	−1
−1	−1	1	1	−1	1	−1	1	−1	1	−1	1
−1	1	−1	−1	−1	1	1	−1	−1	1	1	1
−1	1	−1	1	1	−1	1	−1	1	1	−1	−1
−1	1	1	−1	1	1	1	1	1	−1	−1	1
−1	1	1	1	−1	−1	1	1	−1	−1	1	−1
1	−1	−1	−1	−1	1	1	1	1	−1	1	−1
1	−1	−1	1	1	−1	1	1	−1	−1	−1	1
1	−1	1	−1	1	1	1	−1	−1	1	−1	−1
1	−1	1	1	−1	−1	1	−1	1	1	1	1
1	1	−1	−1	−1	−1	−1	1	1	1	−1	1
1	1	−1	1	1	1	−1	1	−1	1	1	−1
1	1	1	−1	1	−1	−1	−1	−1	−1	1	1
1	1	1	1	−1	1	−1	−1	1	−1	−1	−1

4.4 Maximin distance optimality

The Hamming distance between two rows in a design is the number of positions where they differ. For two-level designs, the L_2-distance and the Hamming distance are equivalent. Using all the Hamming distances of a design, Xu [30] introduced a criterion equivalent to the minimum G_2-aberration criterion, namely, the minimum moment aberration criterion. The idea of [30] offers some insights with respect to finding good space-filling designs under the maximin L_2-distance criterion by the rotation method.

Theorem 4.10. *Suppose that D is an $\mathrm{OA}(\lambda 2^{2^u}, k2^u, 2, t)$ with $t \geqslant 2$ satisfying the condition in Lemma 4.1. Let E be the orthogonal U-type (n, s^m) design with $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ and $m = k2^{u+v}$ $(v = 0, 1, 2, \ldots)$ constructed using D by the rotation method. We have*

$$d(E) = (s^2 - 1)2^v d(D)/3$$

and

$$d_{\text{eff}}(E) \geqslant (n-1)d(D)/(nk2^{u-1}).$$

Theorem 4.10 shows that a two-level orthogonal array D with the larger Hamming distance in the rotation method guarantees a better orthogonal design under the maximin L_2-distance criterion. This also agrees with the findings in the previous subsection. By the connection between the Hamming distance distribution and the generalized wordlength pattern [30], a minimum G_2-aberration design tends to be a maximin Hamming distance design. Therefore, we propose to use minimum G_2-aberration designs as initial orthogonal arrays in the rotation method.

A design D is called mirror-symmetric if the reflection of D about the origin is itself. Applying Theorem 4.10 to some special minimum G_2-aberration orthogonal arrays obtains the following corollary.

Corollary 4.11. *The following U-type (n, s^m) designs or $\mathrm{LHD}(n, m)$s, denoted by E, can be constructed using orthogonal arrays D by the rotation method.*

(i) *If D is an $\mathrm{OA}(4\lambda, 4\lambda - 2, 2, 2)$ obtained by deleting one column of a saturated two-level orthogonal array, then orthogonal U-type designs E with $n = \lambda 2^{v+2}$, $s = 2^{v+2}$ and $m = (2\lambda - 1)2^{v+1}$ $(v = 0, 1, 2, \ldots)$ can be constructed. Furthermore, $d(E) = (2\lambda - 1)(s^2 - 1)2^v/3$ and $d_{\text{eff}}(E) \geqslant 1 - 1/n \to 1$ as $n \to \infty$.*

(ii) *If D is an $\mathrm{OA}(\lambda 2^{2^u}, \lambda 2^{2^u-1}, 2, 3)$ satisfying the condition in Lemma 4.1, then orthogonal U-type designs E with $n = \lambda 2^{2^u+v}$, $s = 2^{2^u+v}$ and $m = \lambda 2^{2^u+v-1}$ $(v = 0, 1, 2, \ldots)$ can be constructed. Furthermore,*

(a) *E is mirror-symmetric and 3-orthogonal;*

(b) $d(E) = \lambda(s^2-1)2^{2^u+v-2}/3$, $d_{\text{eff}}(E) \geqslant 1-1/n \to 1$ *as* $n \to \infty$, *and* E *is an exact maximin distance design among all the mirror-symmetric U-type* (n, s^m) *designs.*

(iii) *If* D *is the* OA$(16, 8, 2, 3)$ *given by* (D_1, D_4) *in Example* 4.8, *then orthogonal* LHD(n, m)*s* E *with* $n = 2^{v+4}$ *and* $m = 2^{v+3}$ $(v = 0, 1, 2, \ldots)$ *can be constructed. Furthermore,* $d(E) = (2^{2v+8}-1)2^{v+2}/3$ *and* $d_{\text{eff}}(E) \geqslant 1-1/n = 1-2^{-v-4} \to 1$ *as* $n \to \infty$.

(iv) *If* D *is the* OA$(16, 12, 2, 2)$ *given in Table* 4, *then orthogonal* LHD(n, m)*s* E *with* $n = 2^{v+4}$ *and* $m = 3 \cdot 2^{v+2}$ $(v = 0, 1, 2, \ldots)$ *can be constructed. Furthermore,* $d(E) = (2^{2v+8}-1)2^{v+1}$ *and* $d_{\text{eff}}(E) \geqslant 1-1/n = 1-2^{-v-4} \to 1$ *as* $n \to \infty$.

Remark 4.12. (i) The orthogonal arrays D in (i)–(iv) of Corollary 4.11 all have minimum G_2-aberration by [3, Theorem 3].

(ii) The 3-orthogonal LHD E in Example 4.8 corresponds to the special case of Corollary 4.11(iii) with $v = 0$. By [27], all the 3-orthogonal LHDs in Corollary 4.11(iii) are exact maximin distance designs among all the mirror-symmetric LHD$(2^{v+4}, 2^{v+3})$s for $v = 0, 1, 2, \ldots$ Orthogonal LHDs of the same sizes as in Corollary 4.11(iii) can also be obtained by the method of [21] or by using an OA$(4, 2, 2, 2)$, i.e., a full factorial of 4 runs and 2 factors, as D in the rotation method. One can check that all of them are 3-orthogonal LHDs with the same L_2-distance distributions.

(iii) The LHD$(16, 12)$ E^* in Example 4.9 corresponds to the special case of Corollary 4.11(iv) with $v = 0$.

Corollary 4.11 constructs several infinite families of orthogonal or 3-orthogonal U-type designs which also perform well under the maximin distance criterion. Table 5 shows some small-sized orthogonal U-type (n, s^m) designs with $n = \lambda s$ and $\lambda \leqslant 4$ as rotated minimum G_2-aberration designs. The cases of $\lambda = 1$ correspond to LHDs. We see that all of these designs have large distance efficiencies.

In addition to Table 5, there are many other sources of minimum G_2-aberration orthogonal arrays that can be used as D in the rotation method. Butler presented over 80 minimum G_2-aberration orthogonal arrays with run sizes n equaling 16, 24, 32, 48, 64 and 96 (see [3, Table 1]). For example, when $n = 48$, such designs are available with m equaling 22–26, 35–38, 40–42 and 44–47. All of these designs or their subarrays with an even number of columns can be used in the rotation method. It is also worth noting that the minimum G_2-aberration criterion is a special case of the generalized minimum aberration criterion proposed by [28]. More algebraic and algorithmic constructions of optimal or nearly-optimal large-sized orthogonal arrays under the minimum G_2-aberration criterion can be found in [31] and the references therein.

Table 5 Some small-sized maximin distance orthogonal U-type (n, s^m) designs with $n = \lambda s$ and $\lambda \leqslant 4$

λ	n	s	m	Rotation matrix	$d(E)$	$d_{\text{eff}}(E)$	3-orthogonal	Source
1	4		2	R_{10}	5	0.833	Yes	Corollary 4.11(i) or Corollary 4.11(ii)
1	8		4	R_{11}	42	0.875	Yes	Corollary 4.11(i) or Corollary 4.11(ii)
1	16		8	R_{12}	340	0.939	Yes	Corollary 4.11(iii)
1	16		12	R_{20}	510	0.938		Corollary 4.11(iv)
1	32		16	R_{13}	2,728	0.969	Yes	Corollary 4.11(iii)
1	32		24	R_{21}	4,092	0.969		Corollary 4.11(iv)
2	8	4	4	R_{10}	10	0.909	Yes	Corollary 4.11(ii)
2	8	4	6	R_{10}	15	0.882		Corollary 4.11(i)
2	16	8	8	R_{11}	84	0.944	Yes	Corollary 4.11(ii)
2	16	8	12	R_{11}	126	0.940		Corollary 4.11(i)
3	12	4	10	R_{10}	25	0.926		Corollary 4.11(i)
3	24	8	20	R_{11}	210	0.959		Corollary 4.11(i)
4	16	4	8	R_{10}	20	0.952	Yes	Corollary 4.11(ii)
4	16	4	14	R_{10}	35	0.946		Corollary 4.11(i)
4	32	8	16	R_{11}	168	0.971	Yes	Corollary 4.11(ii)
4	32	8	28	R_{10}	294	0.970		Corollary 4.11(i)

Table 6 $d_{\rm eff}$ values (the larger the better) and ρ^2 values (the smaller the better) of different LHD(n,m)s

	(n,m)	$(8,4)$	$(16,8)$	$(16,12)$	$(32,16)$	$(32,24)$
$d_{\rm eff}$	SLHD	**0.875**	0.770	0.858	0.806	0.902
	OM	**0.875**	0.729	0.803	0.715	0.807
	Rotation	**0.875**	**0.939**	**0.938**	**0.969**	**0.969**
$10^2\rho^2$	SLHD	**0.000**	0.538	1.222	0.365	0.568
	OM	**0.000**	0.089	0.072	0.042	0.070
	Rotation	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**

Below we compare the obtained LHDs of sizes (n,m) equaling $(8,4)$, $(16,8)$, $(16,12)$, $(32,16)$ and $(32,24)$ with designs of the same sizes generated by two standard methods under the orthogonality and maximin L_2-distance criteria. The first are maximin LHDs produced by the R package SLHD [1] and the second are orthogonal-maximin (OM) LHDs achieved by the simulated annealing algorithm in [10]. Each algorithm was run 100 times with default settings, and the best design was selected. For the orthogonal-maximin algorithm, the L_2-distance was used, and the weight parameter was set to $w=0.5$. Table 6 shows the $d_{\rm eff}$ and ρ^2 values of these designs, where "Rotation" denotes the design obtained by the rotation and bold fonts represent the best results. We see that expect for the case of $(n,m)=(8,4)$ where the three methods generate the same design, the designs obtained by the rotation are the best under both $d_{\rm eff}$ and ρ^2 measures.

5 Application and comparison

This section provides an application of the proposed design method to a computer experiment. We use a 24-dimensional function modified from [14] as the computer simulation code. The output y is determined by

$$y(\boldsymbol{x}) = y_1^*(x_1,\ldots,x_8) + y_2^*(x_9,\ldots,x_{18}) + y_3^*(x_{19},\ldots,x_{24}), \tag{5.1}$$

where $\boldsymbol{x}\in\mathbb{R}^{24}$, $y_i^*=(y_i-\min y_i)/(\max y_i-\min y_i)$, $i=1,2,3$ and

$$y_1(x_1,\ldots,x_8) = \frac{2\pi x_3(x_4-x_6)}{\ln(x_2/x_1)[1+2x_3x_7/(\ln(x_2/x_1)x_1^2x_8)+x_3/x_5]},$$

$$y_2(x_9,\ldots,x_{18}) = 0.036x_9^{0.758}x_{10}^{0.0035}\left(\frac{x_{11}}{\cos^2 x_{12}}\right)^{0.6}x_{13}^{0.006}x_{14}^{0.04}\left(\frac{100x_{15}}{\cos x_{12}}\right)^{-0.3}(x_{16}x_{17})^{0.49}+x_9x_{18},$$

$$y_3(x_{19},\ldots,x_{24}) = \frac{(\frac{12x_{20}}{x_{19}+x_{20}}+0.74)x_{24}(x_{23}+9)}{x_{24}(x_{23}+9)+x_{21}} + \frac{11.35x_{21}}{x_{24}(x_{23}+9)+x_{21}} + \frac{0.74x_{21}x_{24}(x_{23}+9)}{[x_{24}(x_{23}+9)+x_{21}]x_{22}}.$$

Here, $y_1(\cdot)$ is the borehole function with 8 inputs, $y_2(\cdot)$ is an aircraft wing function with 10 inputs, and $y_3(\cdot)$ is an output transformerless (OTL) circuit function with 6 inputs. These functions have been frequently used by [6] and many others, and more details can be found in [14].

We evaluate the performance of the constructed LHD$(32,24)$ in Table 5 by the rotation method in building statistical surrogate models. Four other types of space-filling designs with 32 rows and 24 columns are compared: (i) the maximin LHD$(32,24)$ used in Table 6 generated by the R package SLHD [1]; (ii) the orthogonal-maximin LHD$(32,24)$ used in Table 6 generated by the simulated annealing algorithm in [10]; (iii) a 32-level uniform design generated by the R package UniDOE [32]; (iv) a maximum projection design generated by the R package MaxPro [9]. For each design, we first rescale its levels to $[0,1]$. Next, we conduct permutations on column labels and reflections within columns for a random subset of inputs. Then we use the design points as inputs to generate the responses by evaluating the function (5.1). Finally, we fit a universal kriging model with the linear trends and Gaussian correlation function, i.e., the model (1.1) with $p=2$, to approximate the true function (5.1).

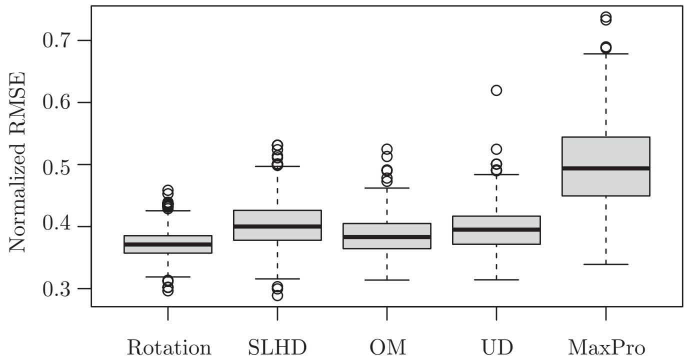

Figure 1 Box plots of normalized RMSEs for the constructed LHD(32, 24) (Rotation), the maximin LHD(32, 24) (SLHD), the orthogonal-maximin LHD(32, 24) (OM), the uniform design (UD) and the maximum projection design (MaxPro)

To judge predictor performance, a random LHD(N, 24) with $N = 10^5$ is used as the test data and the normalized root mean squared error (RMSE), i.e.,

$$\text{Normalized RMSE} = \sqrt{\frac{N^{-1}\sum_{i=1}^{N}(\hat{y}(\boldsymbol{x}_i) - y(\boldsymbol{x}_i))^2}{N^{-1}\sum_{i=1}^{N}(\bar{y} - y(\boldsymbol{x}_i))^2}},$$

is used as the statistical performance measure. Here, $\hat{y}(\cdot)$ is the fitted kriging model, $\boldsymbol{x}_i$ ($i = 1, \ldots, N$) are the test data points, and $\bar{y}$ is the mean response of the data used to build the kriging model. Figure 1 shows the box plots of normalized RMSEs for each design over 500 random permutations and reflections. We see that the LHD(32, 24) (Rotation) constructed by the proposed rotation method outperforms the other designs. This meets our expectations as the constructed design is strictly orthogonal ($\rho^2 = 0$) and has the largest distance efficiency in Table 6. These properties, as shown by [10] in terms of the maximum entropy criterion, can improve the performance of the kriging predictor (1.1).

6 Concluding remarks

The rotation method is powerful for constructing orthogonal designs. Based on the connections between the initial two-level orthogonal arrays and their rotations, we show some maximin distance properties of the orthogonal designs by the rotation method. To acquire better orthogonal and 3-orthogonal designs under the maximin distance criterion, we propose to use minimum G_2-aberration fractional factorial designs as initial designs. Several new families of orthogonal-maximin designs are constructed, and an application of the design is given. The obtained designs are particularly suitable for building statistical surrogate models in computer experiments.

Note that the rotation method in [23] can also be applied to s-level orthogonal arrays where $s > 2$, and it would be natural to ask whether the similar properties to those in the two-level case hold for the s-level case. Unfortunately, under the distance variance criterion, numerical examples indicate that the orthogonal design via rotating an s-level orthogonal array is not necessarily optimal. Under the ϕ_q and maximin L_2-distance criteria, it is also difficult to build direct links between the Hamming distance of the initial orthogonal array and the L_2-distance of the final design as in the two-level case. The issue of how to choose appropriate orthogonal arrays for the s-level case will be an interesting topic for future research.

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Appendix A Proofs

Proof of Lemma 4.1. If D has strength two, then the result follows by a similar argument of [23]. If D has strength three, then it is well known that D^v, i.e., the v-time double of D defined in (4.1), is also a strength three orthogonal array. Hence, it follows from [22, Theorem 1] that $E = D^vR$ is 3-orthogonal, where $R = I_k \otimes R_{uv}$. □

To prove Theorem 4.2, we need the following two lemmas which are due to [26].

Lemma A.1. *For a U-type* (n, s^m) *design* $D = (x_{ik})$ *and any* $i = 1, \dots, n$,

$$\sum_{j=1}^{n} d(\boldsymbol{x}_i, \boldsymbol{x}_j) = nm(s^2-1)/12 + nd(\boldsymbol{x}_i, 0). \tag{A.1}$$

Lemma A.2. *For a U-type* (n, s^m) *design* $D = (x_{ik})$, *we have*

$$\rho^2(D) = 36[n^2m(m-1)(s^2-1)^2]^{-1}h(D) + 1, \tag{A.2}$$

where

$$h(D) = \sum_{i=1}^{n}\sum_{j=1}^{n} d^2(\boldsymbol{x}_i, \boldsymbol{x}_j) - 2n^{-1}\sum_{i=1}^{n}\left[\sum_{j=1}^{n} d(\boldsymbol{x}_i, \boldsymbol{x}_j)\right]^2.$$

Proof of Theorem 4.2. Equation (4.2) follows from substituting (2.1) and (A.1) into (A.2) and some algebra. It remains to show (4.3). By (4.2), $V(D)$ is minimized if $\rho^2(D)$ and $\sum_{i=1}^n d^2(\boldsymbol{x}_i, 0)$ are simultaneously minimized. A lower bound of $\rho^2(D)$ is zero and is attained if and only if D is orthogonal. A lower bound of $\sum_{i=1}^n d^2(\boldsymbol{x}_i, 0)$ is also easy to obtain using the Cauchy-Schwarz inequality. The level balance property implies that

$$\sum_{i=1}^{n} d(\boldsymbol{x}_i, 0) = nm(s^2-1)/12,$$

and hence,

$$\sum_{i=1}^{n} d^2(\boldsymbol{x}_i, 0) \geqslant n^{-1}\left(\sum_{i=1}^{n} d(\boldsymbol{x}_i, 0)\right)^2 = nm^2(s^2-1)^2/144$$

with the equality holding if and only if $d(\boldsymbol{x}_i, 0) = m(s^2-1)/12$ for any $1 \leqslant i \leqslant n$. By the above two bounds, the result is proved. □

Proof of Theorem 4.5. Let $D_0 = (x_{ij})$ be an $(n_0, 2^{m_0})$ design and $\tilde{D}_0 = (\tilde{x}_{i'j'})$ be the double of D. Then $\tilde{D}_0$ is a $(2n_0, 2^{2m_0})$ design and it is easy to verify that for $1 \leqslant i' < j' \leqslant 2n_0$,

$$d(\tilde{\boldsymbol{x}}_{i'}, \tilde{\boldsymbol{x}}_{j'}) = \begin{cases} 2d(\boldsymbol{x}_{i'}, \boldsymbol{x}_{j'}), & 1 \leqslant i' < j' \leqslant n_0, \\ 2d(\boldsymbol{x}_{i'-n_0}, \boldsymbol{x}_{j'-n_0}), & n_0+1 \leqslant i' < j' \leqslant 2n_0, \\ m_0, & \text{otherwise}. \end{cases} \tag{A.3}$$

In the rotation method, the design D^v in (4.1) is the column juxtaposition of D_j^v ($j = 1, \dots, k$), and each D_j^v is obtained by iteratively doubling each D_j v times. Therefore, from (A.3), we know that the distance distributions of D^v, and correspondingly, $E = D^vR$, are both completely determined by the initial orthogonal array $D = (x_{ij})$, where $R = I_k \otimes R_{uv}$. More specifically, among all the $\binom{n}{2}$ distances in D^v,

$$\binom{n}{2} - 2^v\binom{n/2^v}{2}$$

of them take the value $m/2$, and the remaining

$$2^v\binom{n/2^v}{2}$$

of them repeat each of the values $2^v d(\boldsymbol{x}_i, \boldsymbol{x}_j)$ $(1 \leqslant i < j \leqslant n/2^v)$ 2^v times.

Based on the above argument, we have

$$\begin{aligned}\phi_q(D^v) &= \binom{n}{2}^{-1}\left[2^v \sum_{1\leqslant i<j\leqslant n/2^v} q^{2^v d(\boldsymbol{x}_i,\boldsymbol{x}_j)} + \left(\binom{n}{2} - 2^v\binom{n/2^v}{2}\right)q^{m/2}\right] \\ &= \frac{n/2^v - 1}{n-1}\phi_{q^{2^v}}(D) + \frac{n - n/2^v}{n-1}q^{m/2}.\end{aligned}$$

Finally, the conclusion follows by $R^{\mathrm{T}}R = \alpha I_m$ and

$$\phi_q(E) = \phi_q(D^v R) = \phi_{q^\alpha}(D^v),$$

where $\alpha = (2^{2^{u+1}+2v} - 1)/3 = (s^2-1)/3$. □

Proof of Corollary 4.7. For an $(n, 2^m)$ design D, let $\mathcal{U}$ be a subset of column indices $1, \ldots, m$. The J-characteristic of the corresponding columns in $\mathcal{U}$ is defined by $J_{\mathcal{U}} = \sum_{i=1}^n \prod_{k\in\mathcal{U}} x_{ik}$. Then by [5], $A_i(D)$ can be represented by using J-characteristics as

$$A_i(D) = n^{-1}\sum_{|\mathcal{U}|=i} |J_{\mathcal{U}}|^2.$$

This implies that

$$0 \leqslant A_i(D) \leqslant \binom{m}{i}$$

and $n^2 A_i(D)$ is a nonnegative integer for $1 \leqslant i \leqslant m$. Therefore, there exists a positive integer

$$M = \binom{m}{\lfloor m/2\rfloor}$$

such that $0 \leqslant A_i(D) \leqslant M$ for any $1 \leqslant i \leqslant m$.

For two $(n, 2^m)$ designs D and D', suppose that D has less generalized aberration than D', i.e., there exists some $1 \leqslant j \leqslant m$ such that $A_i(D) = A_i(D')$ for $1 \leqslant i \leqslant j-1$ and $A_j(D) < A_j(D')$. We then have

$$1 \leqslant n^2 A_j(D') - n^2 A_j(D) \leqslant n^2 M$$

and

$$\begin{aligned}\phi_q(D') - \phi_q(D) &= (n-1)^{-1} n\left(\frac{1+q}{2}\right)^m \sum_{i=j}^m \left(\frac{1-q}{1+q}\right)^i (A_i(D') - A_i(D)) \\ &= [n(n-1)]^{-1}\left(\frac{1-q}{2}\right)^m \sum_{i=j}^m \left(\frac{1+q}{1-q}\right)^{m-i} (n^2 A_i(D') - n^2 A_i(D)).\end{aligned}$$

The condition $n^2M/(n^2M+2) \leqslant q < 1$ is equivalent to $(1+q)/(1-q) \geqslant n^2M + 1$. Therefore,

$$\begin{aligned}&\sum_{i=j}^m \left(\frac{1+q}{1-q}\right)^{m-i}(n^2 A_i(D') - n^2 A_i(D)) \\ &\quad\geqslant \left(\frac{1+q}{1-q}\right)^{m-j} - \sum_{i=j+1}^m \left(\frac{1+q}{1-q}\right)^{m-i} n^2 M \\ &\quad\geqslant \left(\frac{1+q}{1-q}\right)^{m-j} - \sum_{i=j+1}^m \left(\frac{1+q}{1-q}\right)^{m-i}\left(\frac{1+q}{1-q} - 1\right) = 1,\end{aligned}$$

which implies $\phi_q(D') - \phi_q(D) > 0$. Conversely, it is also easy to verify that if $(1+q)/(1-q) \geqslant n^2M+1$, then $\phi_q(D') - \phi_q(D) > 0$ implies that D has less generalized aberration than D'. The conclusion follows. □

Proof of Theorem 4.10. Let $D = (x_{ij})$. From the proof of Theorem 4.5 we know that among all the $\binom{n}{2}$ distances in E,

$$\binom{n}{2} - 2^v \binom{n/2^v}{2}$$

of them take the value $m(s^2 - 1)/6$, and the remaining $2^v \binom{n/2^v}{2}$ of them repeat each of the values $2^v(s^2 - 1)d(\boldsymbol{x}_i, \boldsymbol{x}_j)/3$ $(1 \leqslant i < j \leqslant n/2^v)$ 2^v times. The result then follows from Lemma 2.1 and the fact that for a two-level orthogonal array of strength two, $d(\boldsymbol{x}_i, \boldsymbol{x}_j) \leqslant m/2^{v+1}$ $(1 \leqslant i < j \leqslant n/2^v)$. □

To prove Corollary 4.11, we need the following two lemmas. Lemma A.3 is [4, Theorem 3] and Lemma A.4 is [27, Theorem 1].

Lemma A.3. *Foldover designs are the only (regular or nonregular) two-level factorial designs of strength three or more with $n/3 \leqslant m \leqslant n/2$ factors.*

Lemma A.4. *Let $D = (X^{\mathrm{T}}, -X^{\mathrm{T}})^{\mathrm{T}}$ be a mirror-symmetric U-type (n, s^m) design with $n = 2m$.*

(i) *If D is orthogonal, then D has the maximin L_2-distance among all the mirror-symmetric U-type (n, s^m) designs.*

(ii) *If D has the maximin L_2-distance with $d_2(D) = (s^2 - 1)m/6$, then D is orthogonal.*

Proof of Corollary 4.11. (i) It is well known that a saturated two-level orthogonal array, say, $\mathrm{OA}(4\lambda, 4\lambda - 1, 2, 2)$, is Hamming equidistant with the distance 2λ. Because D is obtained by deleting one column of an $\mathrm{OA}(4\lambda, 4\lambda - 1, 2, 2)$, we must have $d(D) = 2\lambda - 1$. The result then follows from Theorem 4.10.

(ii) Because D has strength three, by Lemma A.3, D must be mirror-symmetric. This also means that $d(D) = \lambda 2^{2^u - 2}$ by Lemma A.4. Part (i) then follows from Lemma 4.1. Part (ii) follows from Lemma A.4 and Theorem 4.10.

(iii) The result follows directly from (i) or (ii).

(iv) The result follows from $d(D) = 6$, Theorem 4.10 and the fact that $\bar{d}$ (referring to (2.1)) is an integer for E. □