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NONREGULAR DESIGNS FOR QUANTITATIVE FACTORS

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Abstract: Fractional factorial designs are widely used to design screening experiments. Nonregular fractional factorial designs can have better properties than regular designs, but their construction is challenging. Current research on the construction of nonregular designs focuses on two-level designs. We provide a novel class of multilevel nonregular designs by permuting levels of regular designs. We develop a theory illustrating how levels can be permuted without a computer search and, accordingly, propose a sequential method for constructing nonregular designs. Compared with regular designs, these nonregular designs provide more accurate estimations on factorial effects and more efficient screening for experiments with quantitative factors. We further explore the space-filling property of the obtained designs and demonstrate their superiority.

Key words and phrases: Generalized minimum aberration, geometric isomorphism, level permutation, orthogonal array, regular design, Williams transformation.

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1. Introduction

Screening experiments are commonly designed to investigate controlled factors and identify which of them are important. Fractional factorial designs are highly suitable for screening experiments because they allow us to investigate many factors simultaneously using a small number of runs. These designs are classified into two broad types: regular designs and nonregular designs. Designs that can be constructed by defining relations between factors are called regular designs; all other designs are nonregular. There are many more nonregular designs than there are regular designs. Good nonregular designs can either fill the gaps between regular designs in terms of various run sizes, or provide better estimations for factorial effects.

The construction of good nonregular designs is important and challenging. Constructions for two-level nonregular designs have been presented by Plackett and Burman (1946), Deng and Tang (2002), Xu and Deng (2005), Fang et al. (2007), and Phoa and Xu (2009), among others. While numerous constructions are available for two-level designs, these designs are not able to provide information on quadratic or higher order factorial effects. Multilevel designs with three or more levels are useful in many scientific and engineering fields, such as drug combination experiments (Ding et al., 2013; Jaynes et al., 2013; Silva et al., 2016; Clemens et al., 2019), because

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these designs enable researchers to study complex factorial effects and interactions. They are also flexible in terms of the number of levels for factors, without the strict restriction on Latin hypercube designs (LHDs) that the number of levels has to be the same as the run size. Nevertheless, there are very few constructions for multilevel nonregular designs (Xu et al., 2009), because the large number of such designs makes providing an efficient algorithm for searching the design space extremely challenging. A systematic construction also seems impossible without a unified mathematical description.

This study provides a class of multilevel nonregular designs by manipulating nonlinear-level permutations on regular designs. Although linear-level permutations have been studied by Cheng and Wu (2001), Xu et al. (2004), and Ye et al. (2007) for three-level designs, and Tang and Xu (2014) have improved the properties of regular designs, nonlinear level permutations have not been studied. Note that linearly permuted regular designs can be still considered as regular because they are just cosets of regular designs and share the same defining relationship. We consider a nonlinear-level permutation based on the Williams transformation, which was first used by Williams (1949) to construct balanced Latin square designs, and then by Butler (2001) and Wang et al. (2018b) to construct orthogonal or

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maximin LHDs. However, our purpose differs from theirs. We provide a class of nonregular designs by manipulating nonlinear-level permutations on regular designs using the Williams transformation, and develop a general theory on the obtained designs. Using this theory, we propose a sequential construction method that efficiently constructs good designs in terms of the minimum β-aberration criterion, which is used to assess multilevel designs. We further explore the space-filling property of the obtained designs and demonstrate their superiority.

The remainder of the paper is organized as follows. Section 2 introduces the minimum β-aberration criterion and generates a class of nonregular designs using the Williams transformation. Section 3 presents our main theoretical results. Based on the theory, in Section 4, we propose a sequential construction method and compare the constructed designs with available designs. In Section 5, we apply the constructed designs. Section 6 concludes the paper. All proofs are deferred to the Appendix.

2. Notation, Background, and Definitions

Let $Z_q = \{0, \ldots, q-1\}$. A q-level design $D = (x_{ij})$ with N runs and n factors is an $N \times n$ matrix over Z_q, where each column corresponds to a factor. Let $p_0(x) \equiv 1$ and $p_j(x)$, for $j = 1, \ldots, q-1$, be an orthonormal

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polynomial of order j defined on Z_q, satisfying

$$\sum_{x=0}^{q-1} p_i(x)p_j(x) = \begin{cases} 0, & i \neq j; \\ q, & i = j. \end{cases}$$

The set $\{p_0(x), p_1(x), \ldots, p_{q-1}(x)\}$ is called an orthonormal polynomial basis.

Multilevel designs are often used to study quantitative factors by fitting response surface models such as polynomial models. A commonly accepted principle for polynomial models is that the effects of a lower polynomial order are more important than those of a higher polynomial order, while the effects of the same polynomial order are regarded as equally important. Based on this principle, Cheng and Ye (2004) proposed the *minimum β-aberration* criterion for selecting multilevel designs. For a q-level design $D = (x_{ij})$ with N runs and n factors, define

$$\beta_k(D) = N^{-2} \sum_{\|u\|_1 = k} \left| \sum_{i=1}^{N} \prod_{j=1}^{n} p_{u_j}(x_{ij}) \right|^2 \text{ for } k = 1, \ldots, K, \tag{2.1}$$

where $u = (u_1, \ldots, u_n) \in Z_q^n$, $\|u\|_1 = u_1 + \cdots + u_n$, and $K = n(q-1)$. The vector $(\beta_1(D), \ldots, \beta_K(D))$ is called the β-wordlength pattern of D, and each β_k measures the overall aliasing between the jth- and the $(k-j)$th-order polynomial terms, for all j, with $0 \leq j \leq k$. The minimum β-aberration criterion sequentially minimizes β_k, for $k = 1, 2, \ldots, K$. Because linear

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and second-order terms are more important than higher-order terms, the sequential minimization of $\beta_1, \ldots, \beta_4$ is adequate for choosing designs in practice. Tang and Xu (2014) and Lin et al. (2017) provide statistical justifications and additional insights for minimum β-aberration designs.

The minimum β-aberration criterion is an extension of the minimum G_2-aberration criterion (Tang and Deng, 1999) for two-level designs, but differs from the generalized minimum aberration criterion (Xu and Wu, 2001) for multi-level designs with qualitative factors.

For $x \in Z_q$, the Williams transformation is defined by

$$W(x) = \begin{cases} 2x, & \text{for } 0 \leq x < q/2; \\ 2(q-x)-1, & \text{for } q/2 \leq x < q. \end{cases} \tag{2.2}$$

The Williams transformation is a permutation of Z_q. For a design $D = (x_{ij})$, let $W(D) = (W(x_{ij}))$. The following example shows that we can get better designs from the Williams transformation.

Example 1. Consider a five-level regular design D with three columns, x_1, x_2, and $x_3 = x_1 + x_2 \pmod 5$. By (2.1), $\beta_1(D) = \beta_2(D) = 0$, $\beta_3(D) = 0.125$, and $\beta_4(D) = 0.525$. For each $b = 0, \ldots, 4$, we obtain two designs using linear permutations and the Williams transformation, namely, D_b with columns x_1, x_2, and $x_3 = x_1 + x_2 + b \pmod 5$, and $E_b = W(D_b)$. It can be verified that all D_b and E_b have $\beta_1 = \beta_2 = 0$. Table 1 shows their β_3 and β_4. The

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Table 1: The β-wordlength pattern of D_b and E_b in Example 1.

b	$\beta_3(D_b)$	$\beta_4(D_b)$	$\beta_3(E_b)$	$\beta_4(E_b)$
0	0.125	0.525	0.442	0.004
1	0.125	0.525	0.168	0.021
2	0.125	0.096	0.168	0.021
3	0.000	0.686	0.442	0.004
4	0.125	0.096	0.000	0.027

best design from D_b is D_3 with $\beta_3 = 0$ and $\beta_4 = 0.686$, while the best design from E_b is E_4 with $\beta_3 = 0$ and $\beta_4 = 0.027$. Design E_4 performs much better than D_3 under the minimum β-aberration criterion, although both are better than the original design D.

Remark 1. In the computation of β_k defined in (2.1), the orthonormal polynomials for a five-level factor are $p_0(x) = 1$, $p_1(x) = (x-2)/\sqrt{2}$, $p_2(x) = \sqrt{10/7}\{p_1(x)^2 - 1\}$, $p_3(x) = \{10p_1(x)^3 - 17p_1(x)\}/6$, and $p_4(x) = \{70p_1(x)^4 - 155p_1(x)^2 + 36\}/\sqrt{14}$.

Example 1 shows that from a regular design, we can obtain a series of nonregular designs using linear permutations and the Williams transformation. This series provides better designs than those of the original regular design and linearly permuted designs.

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In general, for a prime number q, a regular q^{n-m} design D has $n-m$ independent columns, denoted as $x_1, \ldots, x_{n-m}$, and m dependent columns, denoted as $x_{n-m+1}, \ldots, x_n$, which can be specified by m generators as

$$x_{n-m+i} = c_{i1}x_1 + \cdots + c_{i(n-m)}x_{n-m} \pmod q, \text{ for } i = 1, \ldots, m, \tag{2.3}$$

where each vector $(c_{i1}, \ldots, c_{i(n-m)})$ is a generator with entries that are constants in Z_q. For each regular q^{n-m} design D and $b = (b_1, \ldots, b_m) \in Z_q^m$, let

$$D_b = (x_1, \ldots, x_{n-m}, x_{n-m+1} + b_1, \ldots, x_n + b_m) \pmod q, \tag{2.4}$$

and

$$E_b = W(D_b). \tag{2.5}$$

Note that we only consider permutations for dependent columns in (2.4) because linearly permuting one or more independent columns is equivalent to linearly permuting some dependent columns, which can be seen from (2.3). Throughout the paper, all additions between columns of a design are subject to the modulus q, the number of levels of the design, as in (2.3) and (2.4). We omit the notation $\pmod q$ for such operations when no confusion is introduced. From each regular q^{n-m} design D, we can derive q^m of D_b and q^m of E_b. To find the best design, one can search over all possible permutations $b \in Z_q^m$. However, this is cumbersome and even infeasible in

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many cases. In the next section, we develop a theory to determine the best E_b without employing a computer search.

For $q = 3$, the two classes of designs, D_b and E_b, always have the same β-wordlength patterns because they are geometrically isomorphic (Cheng and Ye, 2004). However, with more than three levels, their performance varies significantly under the minimum β-aberration criterion. Tang and Xu (2014) studied the class of D_b. As we have seen in Example 1, the class of E_b provides many better designs than those of the class of D_b.

3. Theoretical Results

We study the properties of E_b in this section. It is well known that a regular design D is an orthogonal array of strength $t \geq 2$. An orthogonal array is a design in which all q^t level combinations appear equally often in every submatrix formed by t columns. Note that t is often omitted when it is equal to two. Because the Williams transformation is a permutation of $\{0, \ldots, q-1\}$, if $D = (x_{ij})$ is a q-level orthogonal array, then $W(D) = (W(x_{ij}))$ is still an orthogonal array. The following result is from Tang and Xu (2014).

Lemma 1. *For an orthogonal array of strength t, $\beta_k = 0$, for $k = 1, \ldots, t$.*

From the construction in (2.5), E_b is an orthogonal array of the same

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strength as D and D_b. While we use designs of strength two in practice, Lemma 1 guarantees that $\beta_1(E_b) = \beta_2(E_b) = 0$; as such, linear terms are not aliased with the intercept or with each other. Then, we want to minimize $\beta_3(E_b)$ in order to minimize the aliasing between the linear and the second-order terms. The following theorem gives a theoretical permutation b that ensures $\beta_3(E_b) = 0$ so that no aliasing exists between any linear terms and second-order terms.

Theorem 1. *For an odd prime q, let*

$$\gamma = W^{-1}((q-1)/2) = \begin{cases} (q-1)/4, & \text{if } q = 1 \pmod 4; \\ (3q-1)/4, & \text{if } q = 3 \pmod 4. \end{cases} \tag{3.1}$$

Let D be a regular q^{n-m} design generated by (2.3)*, and let E_b be defined by* (2.5)*. Then, $\beta_3(E_{b^*}) = 0$, with $b^* = (b_1^*, \ldots, b_m^*)$, where*

$$b_i^* = \left(1 - \sum_{j=1}^{n-m} c_{ij}\right)\gamma \quad (i = 1, \ldots, m). \tag{3.2}$$

Example 2. Consider a 7^{3-1} design D with $x_3 = x_1 + x_2$. Then, $\gamma = (3 \times 7 - 1)/4 = 5$, and equation (3.2) gives $b_1^* = 2$. It can be verified that $\beta_3(E_2) = 0$ and $\beta_4(E_2) = 0.003$. Consider another 7^{3-1} design D with $x_3 = 2x_1 + 2x_2$. Then, $\gamma = 5$, and equation (3.2) gives $b_1^* = 6$. It can be verified that $\beta_3(E_6) = 0$ and $\beta_4(E_6) = 0.0196$.

Theorem 1 states that given a regular design D, we can always find an

E_{b^*} such that $\beta_3(E_{b^*}) = 0$. In the following, we give a sufficient condition for the E_{b^*} to be the unique design with $\beta_3 = 0$ among all possible q^m E_b.

Definition 1. Let D be a regular q^{n-m} design. If there exist $n-m$ independent columns of D, $z_1, \ldots, z_{n-m}$, and a series of $s+1$ sets of columns, $T_0 \subset \cdots \subset T_s$, such that $T_0 = \{z_1, \ldots, z_{n-m}\}$,

$$T_{k+1} = T_k \cup \{w \in D : w = c_1 w_1 + c_2 w_2 \pmod q, w_1, w_2 \in T_k, c_1, c_2 \in Z_q\}, \tag{3.3}$$

for $k = 0, \ldots, s-1$, and $T_s = D$, then D is called recursive. Furthermore, if either c_1 or c_2 is restricted to 1 or -1 in (3.3) for all k, then D is called ordinary-recursive; if both c_1 and c_2 are resticted to 1 or -1 in (3.3) for all k, then D is called simple-recursive.

Example 3. Consider the 7^{3-1} design D defined by $x_3 = 2x_1 + 2x_2$ in Example 2. Clearly, D is recursive. Because $-1 = 6 \pmod 7$, we have $2x_1 + 2x_2 + 6x_3 = 0$, $x_1 + x_2 + 3x_3 = 0$, and $x_2 = -x_1 + 4x_3$. Then, D is also ordinary-recursive if we take $T_0 = \{x_1, x_3\}$ and $T_1 = \{x_1, x_2, x_3\} = D$. However, D is not simple-recursive.

Example 4. Consider a 5^{5-2} design D with $x_4 = x_1 + x_2$ and $x_5 = x_1 + x_2 + x_3$. Take $T_0 = \{x_1, x_2, x_3\}$, $T_1 = \{x_1, x_2, x_3, x_4\}$, and $T_2 = \{x_1, x_2, x_3, x_4, x_5\} = D$. Then, D is simple-recursive. If $x_5 = x_1 + x_2 + 2x_3$

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instead, then D is ordinary-recursive, but not simple-recursive. Consider another 5^{5-2} design D with $x_4 = x_1 + x_2$ and $x_5 = x_1 + 2x_2 + 2x_3$. This design is not recursive because x_5 is not involved in any word of length three. However, when one more column $x_6 = x_1 + 2x_2$ is added, it is ordinary-recursive.

Regular designs with q^2 runs are popular because they are economical and they guarantee that linear terms are uncorrelated. These designs accommodate two independent columns and up to $q-1$ dependent columns. By Definition 1, they are all recursive by letting T_0 include the two independent columns and setting $T_1 = D$.

Lemma 2. *Let q be an odd prime, and let D be a regular design of q^2 runs. Then, D is recursive.*

Clearly, recursive designs include ordinary-recursive designs, which, in turn, include simple-recursive designs. For three-level designs, the three types of designs are equivalent; however, they differ markedly for designs with more than three levels. Table 2 compares the numbers of the three types of designs with 25 and 49 runs. There are far fewer simple-recursive designs than there are other types of designs. Although there is a difference between the numbers of ordinary-recursive and recursive designs, the

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Table 2: The numbers of the three types of recursive designs with 25 and 49 runs.

	25-run designs			49-run designs		
n	simple	ordinary	recursive	simple	ordinary	recursive
3	2	6	8	2	10	18
4	6	22	24	6	99	135
5	20	32	32	20	517	540
6	16	16	16	70	1214	1215
7				252	1458	1458
8				267	729	729

difference is small. As the number of columns increases, all designs tend to be ordinary-recursive.

The next theorem gives a sufficient condition for E_{b^*} to be the unique design with $\beta_3 = 0$ among all possible q^m E_b.

Theorem 2. *For an odd prime q, let D be a regular q^{n-m} design defined by* (2.3)*, and let E_b be defined as in* (2.5)*. If D is ordinary-recursive, then E_{b^*} with b^* defined in* (3.2) *is the only design with $\beta_3 = 0$ among all q^m E_b derived from D.*

In fact, we can show that if D has no more than 13 levels, the result

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of Theorem 2 can be extended beyond ordinary-recursive designs. That is, we have the following more general result for $q \leq 13$.

Theorem 3. *For a recursive q^{n-m} design D, if q is an odd prime and $q \leq 13$, E_{b^*} with b^* defined in (3.2) is the only design with $\beta_3 = 0$ among all E_b derived from D.*

Theorem 3 is not true for $q \geq 17$. A counterexample for $q = 17$ is provided by a 17^{3-1} design with $x_3 = 2x_1 + 4x_2$. By (3.2), $b^* = 14$. Then, E_{14} has $\beta_3 = 0$, while the design E_4 with columns x_1, x_2, and $x_3 + 4$ also has zero β_3. That said, as the number of columns increases, the number of non-ordinary-recursive regular designs decreases dramatically; thus, Theorem 2 works for most recursive designs with many columns.

Example 5. Consider a 7^{8-6} design D with $x_3 = x_1 + x_2, x_4 = x_1 + 2x_2, x_5 = x_1 + 4x_2, x_6 = x_1 + 5x_2, x_7 = 2x_1 + 5x_2$, and $x_8 = 2x_1 + 6x_2$. There are $7^6 = 117,649$ E_b derived from D, which makes it cumbersome, if not impossible, to do an exhaustive search for the best E_b. Note that $x_7 = x_1 + x_6$, and $x_8 = x_3 + x_6$. Therefore, D is ordinary-recursive by taking $T_0 = \{x_1, x_2\}$, $T_1 = \{x_1, \ldots, x_6\}$, and $T_2 = \{x_1, \ldots, x_8\} = D$. Equation (3.2) gives $b_1^* = 2, b_2^* = 4, b_3^* = 1, b_4^* = 3, b_5^* = 5$, and $b_6^* = 0$. It can be verified that $\beta_3(E_{b^*}) = 0$ and $\beta_4(E_{b^*}) = 9.677$. By Theorem 2, E_{b^*} is the

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best design among all E_b derived from D under the minimum β-aberration criterion.

By Theorems 2 and 3, for an ordinary-recursive design or a recursive design with no more than 13 levels, E_{b^*} is the best design among all E_b, which is obtained without a computer search. Theorem 2 does not apply to the class of linearly permuted designs D_b. A counterexample follows.

Example 6. Consider the 7^{3-1} design D defined by $x_3 = 2x_1 + 2x_2$ in Example 2. Example 3 shows that it is ordinary-recursive, but there are three D_b with zero β_3. Specifically, it is easy to verify that $\beta_3(D_b) = 0$ for $b = 0, 3, 5$.

In fact, Tang and Xu (2014) showed that if D is simple-recursive, the design $D_{\tilde{b}}$ given by

$$\tilde{b}_i = \left(1 - \sum_{j=1}^{n-m} c_{ij}\right)(q-1)/2 \quad (i = 1, \ldots, m) \tag{3.4}$$

is the unique design with $\beta_3 = 0$ among all D_b. As we have shown above, only a small number of regular designs are simple-recursive. Therefore, results on simple-recursive designs are usually not applicable for designs with more than three levels. In contrast, Theorem 2 is more general and applies to the broader classes of ordinary-recursive and recursive designs.

Theorem 3 and Lemma 2 indicate the following result.

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Corollary 1. *For an odd prime $q \leq 13$, let D be a regular design of q^2 runs. Then, E_{b^*} with b^* defined as in* (3.2) *is the unique design with $\beta_3 = 0$ among all E_b derived from D.*

Now, we show another useful property of E_{b^*}. A design D over Z_q is called mirror-symmetric if $(q-1)J - D$ is the same design as D, where J is a matrix of unity. Mirror-symmetric designs include two-level foldover designs as special cases.

Theorem 4. *For an odd prime q, let D be a regular q^{n-m} design defined by* (2.3)*, and let E_b be defined as in* (2.5)*. Then, E_{b^*} with b^* defined in* (3.2) *is mirror-symmetric.*

Tang and Xu (2014) showed that a design is mirror-symmetric if and only if it has $\beta_k = 0$ for all odd k. By Theorem 4, E_{b^*} has $\beta_k(E_{b^*}) = 0$ for all odd k. This guarantees that odd-order terms are not aliased with any even-order term. Specifically, linear terms are not aliased with any even-order term.

4. Construction Method and Design Comparisons

Based on our theoretical results, we propose a sequential method for constructing multilevel nonregular designs. For simplicity, we focus on designs with q^2 runs, although the method and results apply to general q^{n-m}

designs. A regular fractional factorial design with q^2 runs has two independent columns, denoted as x_1 and x_2, and can accommodate up to $(q-1)$ dependent columns, each of which is generated by $c_1x_1 + c_2x_2$, with $c_1, c_2 \in \{1, \ldots, q-1\}$. Then, the first two columns of E_{b^*} are $W(x_1)$ and $W(x_2)$, respectively. To obtain $n \geq 3$ columns, we add columns to E_{b^*} sequentially by searching over generators (c_1, c_2). Each new column is generated by $W(c_1x_1 + c_2x_2 + b^*)$, where $b^* = (1 - c_1 - c_2)\gamma$, with γ defined in (3.1) and (c_1, c_2) minimizing $\beta_4(E_{b^*})$; that is,

$$(c_1, c_2) = \arg\min_{(c_1,c_2)} \beta_4(E_{b^*}).$$

The last three columns of Tables 3–5 show the generators of the added columns, as well as the β-wordlength patterns of the obtained E_{b^*}.

To see the merit of E_{b^*}, we compare it with commonly used regular designs and the class of $D_{\tilde{b}}$. The regular design of Mukerjee and Wu (2006), denoted by D, consists of the first n columns of

$$x_1, x_2, x_1 + x_2, x_1 + 2x_2, x_1 + 3x_2, \ldots, x_1 + (q-1)x_2. \tag{4.1}$$

The design $D_{\tilde{b}}$ is obtained sequentially similarly to the generation of E_{b^*}. The only difference is that the added column of $D_{\tilde{b}}$ is $c_1x_1 + c_2x_2 + \tilde{b}$, where $\tilde{b} = (1 - c_1 - c_2)(q-1)/2$. Tables 3–5 compare the obtained designs D, $D_{\tilde{b}}$, and E_{b^*} with 25 runs, 49 runs, and 121 runs, respectively. We can see that

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Table 3: Comparison of β-wordlength patterns for 25-run designs with five levels.

	D		$D_{\tilde{b}}$			E_{b^*}		
n	β_3	β_4	Generators	β_3	β_4	Generators	β_3	β_4
3	0.125	0.525	(1,2)	0	0.271	(1,1)	0	0.027
4	0.375	1.361	(2,1)	0	1.336	(1,2)	0	1.037
5	0.750	3.029	(1,4)	0	3.793	(1,3)	0	3.768
6	1.250	6.786	(1,1)	0	8.250	(2,3)	0	8.250

E_{b^*} always performs best for any design size.

To illustrate the merit of the obtained design E_{b^*}, we further examine its space-filling property. For an $N \times n$ design, we consider the maximin measure in all projection dimensions, which is given by

$$Mm_s = \min_{r=1,\ldots,\binom{n}{s}} \left\{ \frac{1}{\binom{N}{2}} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{d_{ij,sr}^{2s}} \right\}^{-1/(2s)}, \text{ for } s = 1, \ldots, n,$$

where $d_{ij,sr}$ is the Euclidean distance between the ith and jth design points in the rth projection of dimension s. Design points are scaled to $[0,1]^n$ to apply this measure; that is, the jth column is obtained using $x_j/(q-1)$. This measure was proposed in Joseph et al. (2015) to assess the "maximin projection designs." Designs with larger Mm_s values are more space-filling in s-dimension projections. Figure 1 plots the Mm_s values of the 121×12

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Table 4: Comparison of β-wordlength patterns for 49-run designs with seven levels.

	D		$D_{\tilde{b}}$			E_{b^*}		
n	β_3	β_4	Generators	β_3	β_4	Generators	β_3	β_4
3	0.063	0.563	(2,3)	0	0.063	(1,1)	0	0.003
4	0.188	1.354	(1,4)	0	0.313	(3,5)	0	0.055
5	0.375	2.440	(2,5)	0	1.135	(3,6)	0	0.836
6	0.625	4.313	(1,2)	0	3.094	(2,5)	0	2.368
7	0.938	7.401	(2,2)	0	6.438	(2,6)	0	4.928
8	1.312	12.78	(2,6)	0	11.23	(2,3)	0	9.677

designs in Table 5 for $s = 1, \ldots, 12$. We also generate a 121×12 maximum-projection LHD from the R package MaxPro (Joseph et al., 2015), and include its Mm_s values in Figure 1. The design is claimed to be space-filling in all projected dimensions, so can serve as a benchmark in the comparison. Because this design has 121 levels, we further collapse it to an 11-level design and include the Mm_s values of the collapsed design in Figure 1. To obtain a good maximum-projection design, the R package MaxPro is run 100 times and the best design is selected. It takes, on average, seven seconds to get a maximum-projection design. Therefore, to run the package 100 times takes

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Table 5: Comparison of β-wordlength patterns for 121-run designs with 11 levels.

	D		$D_{\tilde{b}}$			E_{b^*}		
n	β_3	β_4	Generators	β_3	β_4	Generators	β_3	β_4
3	0.025	0.585	(2,4)	0	0.010	(1,1)	0	0.0002
4	0.075	1.388	(4,2)	0	0.055	(2,4)	0	0.005
5	0.150	2.350	(5,3)	0	0.281	(4,2)	0	0.015
6	0.250	3.629	(3,5)	0	0.710	(2,9)	0	0.031
7	0.375	5.274	(4,7)	0	1.466	(2,8)	0	0.637
8	0.525	7.682	(1,3)	0	3.152	(5,3)	0	1.308
9	0.700	11.07	(2,8)	0	5.519	(4,10)	0	3.572
10	0.900	15.82	(3,3)	0	8.891	(1,7)	0	5.864
11	1.125	22.26	(1,7)	0	13.49	(5,1)	0	9.896
12	1.375	31.29	(4,10)	0	19.65	(5,4)	0	14.44

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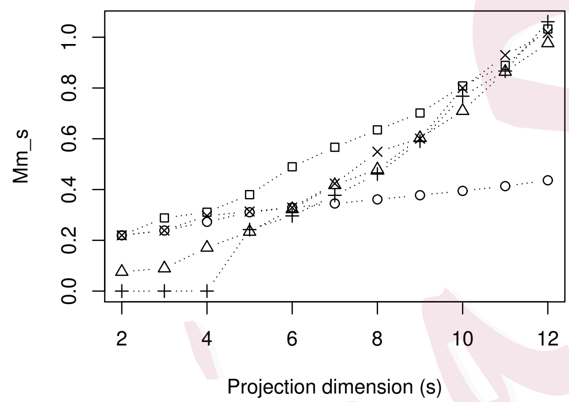
Figure 1: Plot of Mm_s (the larger the better) against s for five designs: D (circle), $D_{\tilde{b}}$ (cross), E_{b^*} (square), the maximum-projection design (triangle), and the collapsed maximum-projection design (plus).



about 12 minutes, whereas it takes less than a second to obtain any of the other designs in the plot. Even so, Figure 1 shows that E_{b^*} outperforms the selected maximum-projection design and its collapsed design for all $s \leq 11$ projection dimensions, although the collapsed design is marginally better than E_{b^*} for the full dimension $s = 12$. In addition, E_{b^*} outperforms all other designs in Figure 1 on projection dimension $s = 2, \ldots, 10$, and is only slightly worse than $D_{\tilde{b}}$ when $s = 11$. The good performance of E_{b^*} comes from its zero β_3 and smaller β_4 values.

We also compare designs of other sizes in Table 5, finding similar per-

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formance. This is because the designs in Table 5 are obtained sequentially, such that those with fewer than 12 columns are actually projections of the 121×12 designs. Therefore, Figure 1 also reflects the projection properties of designs with fewer columns. Similar results hold for 25-run and 49-run designs.

5. Applications

Consider applying the three 25-run designs with three columns and five levels in Table 3 to the following normalized second-order polynomial model:

$$y = \alpha_0 + \sum_{j=1}^{3} p_1(x_j)\alpha_j + \sum_{j=1}^{3} p_2(x_j)\alpha_{jj} + \sum_{j=1}^{2}\sum_{k=j+1}^{3} p_1(x_j)p_1(x_k)\alpha_{jk} + \varepsilon, \quad (5.1)$$

where $p_1(x) = \sqrt{2}(x-2)/2$; $p_2(x) = \sqrt{5/14}\{(x-2)^2 - 2\}$; $\alpha_0, \alpha_j, \alpha_{jj}$, and α_{jk} are the intercept, linear, quadratic, and bilinear terms, respectively; and $\varepsilon \sim N(0, \sigma^2)$. Using this normalized model instead of a model with natural terms (i.e., terms x_j, x_j^2, and $x_j x_k$) produces orthogonality between any two linear terms and between the linear and quadratic terms of an orthogonal array. For the regular design D, because $\beta_3(D) \neq 0$, the linear terms are aliased or correlated with the bilinear terms, and the model in (5.1) is indeed not estimable. Whereas both $D_{\tilde{b}}$ and E_{b^*} have $\beta_1 = \beta_2 = \beta_3 = 0$, the intercept and linear terms are not correlated with the quadratic and bilinear terms, and so they can be estimated independently. For either design, let

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M denote the model matrix corresponding to the three quadratic and three bilinear terms: $\alpha_{11}, \alpha_{22}, \alpha_{33}, \alpha_{12}, \alpha_{13}$, and α_{23}. The variance-covariance matrix of the estimates of the parameters for these terms is $\sigma^2(M^{\mathrm{T}}M)^{-1}$. For $D_{\tilde{b}}$, the variances of the estimates for the quadratic terms, α_{11}, α_{22}, and α_{33}, are $0.047\sigma^2$, $0.041\sigma^2$, and $0.047\sigma^2$, respectively, and for the bilinear terms, α_{12}, α_{13}, and α_{23}, are $0.051\sigma^2$, $0.050\sigma^2$, and $0.051\sigma^2$, respectively. For E_{b^*}, the variance of the estimate for each quadratic term is $0.040\sigma^2$, and that for each bilinear term is $0.041\sigma^2$. With E_{b^*}, the variance of the quadratic terms decreases by up to 14.9%, and the variance of the bilinear terms decreases by up to 19.6%. It can be verified that the correlations between the estimates are also smaller for E_{b^*} than they are for $D_{\tilde{b}}$.

Furthermore, consider the bias brought about by the inadequacy of the polynomial terms in model (5.1). Suppose we have the following nonnegligible third-order polynomial terms:

$$\sum_{i+j+k=3} \alpha_{ijk} p_i(x_1) p_j(x_2) p_k(x_3).$$

Then, the estimates of the linear parameters in model (5.1) are biased by these third-order terms. Specifically, for the estimators from the design $D_{\tilde{b}}$,

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we have

$$E(\hat{\alpha}_1) = \alpha_1 - .12\alpha_{021} - .36\alpha_{012} + .3\alpha_{111},$$

$$E(\hat{\alpha}_2) = \alpha_2 + .36\alpha_{201} - .36\alpha_{102} - .1\alpha_{111},$$

$$E(\hat{\alpha}_3) = \alpha_3 + .36\alpha_{210} - .12\alpha_{120} - .3\alpha_{111},$$

and for the estimators from the design E_{b^*}, we have

$$E(\hat{\alpha}_1) = \alpha_1 + .096\alpha_{021} - .096\alpha_{012} + .08\alpha_{111},$$

$$E(\hat{\alpha}_2) = \alpha_2 + .096\alpha_{201} - .096\alpha_{102} + .08\alpha_{111},$$

$$E(\hat{\alpha}_3) = \alpha_3 + .096\alpha_{210} + .096\alpha_{120} - .08\alpha_{111}.$$

Obviously, the design E_{b^*} brings less bias to the estimators of the linear terms than does $D_{\tilde{b}}$. Because $\beta_5 = 0$ for both designs, the estimates of the second-order terms from $D_{\tilde{b}}$ and E_{b^*} are not biased by third-order terms. In summary, E_{b^*} is better than $D_{\tilde{b}}$ and D_b for screening or studying quantitative factors. The results are general and apply to other designs in Tables 3–5.

6. Conclusion

We provide a new class of nonregular designs based on the Williams transformation, and develop a theory on the property of the obtained designs.

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Using this theory, we further propose a sequential method for constructing nonregular designs with a minimum β-aberration. The sequential method is fast and efficient in terms of generating multilevel nonregular designs using large numbers of runs and factors. Although two-level nonregular designs have been catalogued by some researchers, few works have examined the construction of multilevel nonregular designs. The approach presented here is a pioneering work in this field. The obtained designs provide more accurate estimations on factorial effects and are more efficient than regular designs for screening quantitative factors.

The obtained designs can be used to generate orthogonal LHDs, which are common in computer experiments. Orthogonal LHDs have $\beta_1 = \beta_2 = 0$, thus guaranteeing the orthogonality between the linear effects. A popular construction, proposed by Steinberg and Lin (2006) and Pang et al. (2009), rotates a regular design to obtain an LHD that inherits the orthogonality from both the rotation matrix and the regular design. Wang et al. (2018a) improved the method by rotating a linearly permuted regular design, that is, $D_{\tilde{b}}$, with $\tilde{b}$ defined in (3.4). The orthogonal LHDs generated in this way have $\beta_3 = 0$, and thus guarantee that nonnegligible quadratic and bilinear effects do not contaminate the estimation of the linear effects. Based on the results presented here, we can rotate the class of designs E_{b^*} to obtain new

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orthogonal LHDs that have smaller β_4 values and inherit the good space-filling property of E_{b^*}. These LHDs may be good options for designing computer experiments and Gaussian processing modeling.

The Williams transformation is pairwise linear, which is probably the simplest nonlinear transformation. Nevertheless, it leads to some remarkable results, such as Theorems 2 and 4. It would be of interest to identify and characterize other nonlinear transformations that have similar properties. In addition, the proposed method requires that the number of levels of the regular designs are prime numbers, and does not work for, say, four-level designs. Therefore, it would also be interesting to extend the method to include nonprime numbers of levels.

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Appendix: Proofs of Theorems

We need the following lemmas for the proofs.

Lemma A.1. *The D_b is the same design as $D_e + \gamma \pmod q$, where $e = b - b^*$, γ is defined as* (3.1)*, and b^* is defined as* (3.2)*.*

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Proof. For D_b, permuting all columns x_j to $x_j - \gamma$ for $j = 1, \ldots, n$ is equivalent to keeping the independent columns unchanged while permuting the dependent columns $x_{n-m+i} + b_i$ to $x_{n-m+i} + b_i - b_i^*$ for $i = 1, \ldots, m$. Hence, $D_b - \gamma$ is the same design as D_e with $e = b - b^*$. Equivalently, D_b is the same design as $D_e + \gamma \pmod q$. □

Lemma A.2. *If x is a real number which is not an integer, then*

$$\sum_{n=-\infty}^{\infty} \frac{(-1)^{n-1}}{(n+x)^2} = \frac{\pi^2 \cos \pi x}{(\sin \pi x)^2}.$$

Proof. It is known that $\sum_{n=-\infty}^{\infty} 1/(n+x)^2 = \pi^2/(\sin \pi x)^2$. Then

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} \frac{(-1)^{n-1}}{(n+x)^2} &= \sum_{n=-\infty}^{\infty} \frac{1}{(n+x)^2} - 2 \sum_{\text{even } n} \frac{1}{(n+x)^2} \\
&= \frac{\pi^2}{(\sin \pi x)^2} - \frac{1}{2} \frac{\pi^2}{(\sin(\pi x/2))^2} \\
&= \frac{\pi^2 \cos \pi x}{(\sin \pi x)^2}.
\end{aligned}$$

□

Lemma A.3. *Let $p_1(x) = \rho[x - (q-1)/2]$ be the linear orthogonal polynomial, where $\rho = \sqrt{12/[(q+1)(q-1)]}$. Then for $x = 0, \ldots, q-1$,*

$$p_1(x) = -\frac{\rho}{2q} \sum_{v=0}^{q-1} g(v) \cos\left\{\frac{(2v+1)\pi(x+0.5)}{q}\right\}.$$

where

$$g(v) = \frac{\cos(\pi(v+0.5)/q)}{\{\sin(\pi(v+0.5)/q)\}^2}. \tag{A.1}$$

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Proof. For $x \in (0, q)$, the Fourier-cosine expansion of $x - q/2$ is given by

$$x - \frac{q}{2} = \sum_{v=1}^{\infty} a_v \cos\left(\frac{v\pi x}{q}\right),$$

with

$$a_v = \frac{2}{q}\int_0^q \left(x - \frac{q}{2}\right)\cos\left(\frac{v\pi x}{q}\right)dx = \begin{cases} 0, & \text{if } v \text{ is even;} \\ -4q/(v^2\pi^2), & \text{if } v \text{ is odd.} \end{cases}$$

Then

$$\begin{aligned} p_1(x) &= -\frac{4\rho q}{\pi^2}\sum_{\text{odd } v>0}\frac{1}{v^2}\cos\left(\frac{v\pi(x+0.5)}{q}\right) \\ &= -\frac{2\rho q}{\pi^2}\sum_{v=-\infty}^{\infty}\frac{1}{(2v+1)^2}\cos\left\{\frac{(2v+1)\pi(x+0.5)}{q}\right\} \\ &= -\frac{2\rho q}{\pi^2}\sum_{k=-\infty}^{\infty}\sum_{v=0}^{q-1}\frac{1}{(2kq+2v+1)^2}\cos\left\{\frac{(2kq+2v+1)\pi(x+0.5)}{q}\right\}. \end{aligned}$$

Since for any integers k and x,

$$\cos\left\{\frac{(2kq+2v+1)\pi(x+0.5)}{q}\right\} = (-1)^k\cos\left\{\frac{(2v+1)\pi(x+0.5)}{q}\right\},$$

we have

$$p_1(x) = -\frac{2\rho q}{\pi^2}\sum_{v=0}^{q-1}\sum_{k=-\infty}^{\infty}\frac{(-1)^k}{(2kq+2v+1)^2}\cos\left\{\frac{(2v+1)\pi(x+0.5)}{q}\right\}.$$

By Lemma A.2 and (A.1), we have

$$p_1(x) = -\frac{\rho}{2q}\sum_{v=0}^{q-1} g(v)\cos\left\{\frac{(2v+1)\pi(x+0.5)}{q}\right\}.$$

□

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Proof of Theorem 1. Denote $e = b - b^*$ and $D_e = (y_{ij})$. By Lemma A.1, D_b is the same design as $(D_e + \gamma) \pmod q$, so $E_b = W(D_b) = W(D_e + \gamma)$. By Lemma A.3,

$$\begin{aligned} p_1(W(x)) &= -\frac{\rho}{2q}\sum_{v=0}^{q-1} g(v)\cos\left\{\frac{(2v+1)\pi(W(x)+0.5)}{q}\right\} \\ &= -\frac{\rho}{2q}\sum_{v=0}^{q-1} g(v)\cos\left\{\frac{(2v+1)\pi(2x+0.5)}{q}\right\} \end{aligned}$$

because $\cos\{(2v+1)\pi(W(x)+0.5)/q\} = \cos\{(2v+1)\pi(2x+0.5)/q\}$ for any integer v. Then we have

$$\begin{aligned} \beta_3(E_b) &= \beta_3(W(D_e+\gamma)) \\ &= N^{-2}\sum_{y_1,y_2,y_3}\left|\sum_{i=1}^{N} p_1(W(y_{i1}+\gamma))p_1(W(y_{i2}+\gamma))p_1(W(y_{i3}+\gamma))\right|^2 \\ &= N^{-2}\left(\frac{\rho}{2q}\right)^6 \sum_{y_1,y_2,y_3}\left|\sum_{v_1=0}^{q-1}\sum_{v_2=0}^{q-1}\sum_{v_3=0}^{q-1} g(v_1)g(v_2)g(v_3)S(y,v)\right|^2, \quad \text{(A.2)} \end{aligned}$$

where $\sum_{y_1,y_2,y_3}$ sums over all three different columns y_1, y_2, y_3 in D_e, $y_j = (y_{1j}, \ldots, y_{Nj})$ for $j = 1, 2, 3$, and

$$\begin{aligned} S(y,v) &= \sum_{i=1}^{N}\prod_{j=1}^{3}\cos\left\{\frac{(2v_j+1)\pi(2y_{ij}+2\gamma+0.5)}{q}\right\} \\ &= \sum_{i=1}^{N}\prod_{j=1}^{3}(-1)^{(q+1)/2+v_j}\sin\left\{\frac{2(2v_j+1)\pi y_{ij}}{q}\right\} \\ &= (-1)^{(q+1)/2+v_1+v_2+v_3}\sum_{i=1}^{N}\prod_{j=1}^{3}\sin\left\{\frac{2(2v_j+1)\pi y_{ij}}{q}\right\}. \end{aligned}$$

If $b = b^*$, $e = 0$ and $D_e = D$. Because D is a regular design, it is a linear space over Z_q. Thus, $(q - y_{i1}, \ldots, q - y_{in}) \in D$ whenever $(y_{i1}, \ldots, y_{in}) \in D$.

Then $S(y,v) = 0$ for any $y = (y_1, y_2, y_3)$ and $v = (v_1, v_2, v_3)$. By (A.2), $\beta_3(E_{b^*}) = 0$. $\square$

Proof of Theorem 2. Following the proof of Theorem 1, if $b \neq b^*$, then $e = b - b^*$ has nonzero components. Since D is ordinary-recursive, there exist three columns, say z_1, z_2, z_3, in D such that $z_3 = c_1 z_1 + c_2 z_2$, $c_1 = 1$ or -1, $c_2 \in Z_q$, and z_1, z_2 and $z_3 + e_0$ are three columns in D_e, where e_0 is a nonzero component of e. We only consider $c_1 = 1$ below as the proof for $c_1 = -1$ is similar. Let d be the design formed by z_1, z_2, and $z_3 + e_0$. By (A.2), we only need to show that $\beta_3(W(d)) \neq 0$. Note that

$$\beta_3(W(d)) = N^{-2}\left(\frac{\rho}{2q}\right)^6 \left|\sum_{v_1=0}^{q-1}\sum_{v_2=0}^{q-1}\sum_{v_3=0}^{q-1}(-1)^{v_1+v_2+v_3} g(v_1)g(v_2)g(v_3)S(z,v)\right|^2, \tag{A.3}$$

where $g(v)$ is defined in (A.1), and

$$S(z,v) = \sum_{i=1}^{N} \sin\left(\frac{2(2v_1+1)\pi z_{i1}}{q}\right) \sin\left(\frac{2(2v_2+1)\pi z_{i2}}{q}\right) \sin\left(\frac{2(2v_3+1)\pi(z_{i3}+e_0)}{q}\right).$$

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By applying the product-to-sum identities twice, we have

$$\begin{aligned} S(z,v) \quad &= \frac{1}{4}\Bigg\{ \sum_{i=1}^{N} \sin\left(\frac{2\pi(t_1 z_{i1} - t_4 z_{i2} + (2v_3+1)e_0)}{q}\right) \\ &+ \sum_{i=1}^{N} \sin\left(\frac{2\pi(t_2 z_{i1} + t_4 z_{i2} - (2v_3+1)e_0)}{q}\right) \\ &- \sum_{i=1}^{N} \sin\left(\frac{2\pi(t_1 z_{i1} + t_3 z_{i2} + (2v_3+1)e_0)}{q}\right) \\ &- \sum_{i=1}^{N} \sin\left(\frac{2\pi(t_2 z_{i1} - t_3 z_{i2} - (2v_3+1)e_0)}{q}\right)\Bigg\}, \end{aligned} \tag{A.4}$$

where $t_1 = 2(v_1+v_3)+2$, $t_2 = 2(v_1 - v_3)$, $t_3 = 2(v_2 + v_3 c_2) + c_2 + 1$, and $t_4 = 2(v_2 - v_3 c_2) - c_2 + 1$. Let

$$v_{10} = q - 1 - v_3 \text{ and } v_{20} = v_3 c_2 + (c_2 - 1)(q+1)/2 \pmod{q}. \tag{A.5}$$

When $v_1 = v_{10}$ and $v_2 = v_{20}$, $t_1 = t_4 = 0 \pmod{q}$ and the first item in the right hand side of (A.4), $\sum_{i=1}^{N} \sin(2\pi(t_1 z_{i1} - t_4 z_{i2} + (2v_3+1)e_0)/q)$, equals $N\sin(2\pi(2v_3+1)e_0/q)$. When $v_1 \neq v_{10}$ or $v_2 \neq v_{20}$, the item is zero. By similar analysis to other items in (A.4), we have

$$S(z,v) = \begin{cases} \frac{N}{4}\sin\left\{\frac{2\pi(2v_3+1)e_0}{q}\right\}, & \text{if } (v_1,v_2) = (v_{10}, v_{20}) \text{ or } (q-1-v_{10}, q-1-v_{20}); \\ -\frac{N}{4}\sin\left\{\frac{2\pi(2v_3+1)e_0}{q}\right\}, & \text{if } (v_1,v_2) = (v_{10}, q-1-v_{20}) \text{ or } (q-1-v_{10}, v_{20}); \\ 0, & \text{otherwise.} \end{cases}$$

Note that $g(q-1-v) = -g(v)$ for any v. Then by (A.3),

$$\beta_3(W(d)) = \left(\frac{\rho}{2q}\right)^6 \left|\sum_{v_3=0}^{q-1} (-1)^{v_3 c_2} g(v_{20}) (g(v_3))^2 \sin\left\{\frac{2\pi(2v_3+1)e_0}{q}\right\}\right|^2, \tag{A.6}$$

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where v_{20} is defined in (A.5). Applying $g(q-1-v) = -g(v)$ again, we can simply (A.6) as

$$\beta_3(W(d)) = \frac{\rho^6}{16q^6}\left|\sum_{v_3=0}^{(q-1)/2}(-1)^{v_3c_2}g(v_{20})(g(v_3))^2\sin\left\{\frac{2\pi(2v_3+1)e_0}{q}\right\}\right|^2. \tag{A.7}$$

By considering the Taylor expansion of $g(v)$, we can see that the sum in (A.7) is dominated by the first two items with $v_3 = 0$ and $v_3 = 1$. It can be verified that (A.7) is nonzero for $e_0 = 1, \ldots, q-1$. This completes the proof. $\square$

Proof of Theorem 3. Following the same process as in the proof of Theorem 2, if D is recursive, then for the three columns z_1, z_2, and z_3 in D, $z_3 = c_1z_1 + c_2z_2$, where both c_1 and c_2 can be any value in Z_q. Then we can get (A.4) with t_1 and t_2 replaced by $t_1' = 2(v_1+v_3c_1)+1+c_1$ and $t_2' = 2(v_1-v_3)+1-c_1$, which will in turn result in a change of v_{10} in (A.5) to

$$v_{10}' = \begin{cases} (q-1)/2 - c_1/2 - v_3c_1 \pmod q, & \text{if } c_1 \text{ is an even number;} \\ q - (c_1+1)/2 - v_3c_1 \pmod q, & \text{if } c_1 \text{ is an odd number.} \end{cases}$$

Similar to (A.7), we have

$$\beta_3(W(d)) = \frac{\rho^6}{16q^6}\left|\sum_{v_3=0}^{(q-1)/2}(-1)^{v_3c_2}g(v_{10}')g(v_{20})(g(v_3))\sin\left\{\frac{2\pi(2v_3+1)e_0}{q}\right\}\right|^2. \tag{A.8}$$

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It can be verified that, for $q \leq 13$, (A.8) is nonzero for $e_0 = 1, \ldots, q-1$ for any $c_1, c_2 \in Z_q$. This completes the proof. □

Proof of Theorem 4. We need to show that for any run $W(x_1, \ldots, x_n)$ in E_{b^*}, $(q-1) - W(x_1, \ldots, x_n)$ also belongs to E_{b^*}. This is equivalent to show that for each run $(x_1, \ldots, x_n)$ in D_{b^*}, $W^{-1}(q-1-W(x_1, \ldots, x_n))$ also belongs to D_{b^*}. Since the design D contains the zero point $(0, \ldots, 0)$, by Lemma A.1, D_{b^*} contains the point $(\gamma, \ldots, \gamma)$. Because all design points of D form a linear space and D_b is a coset of D, then $\gamma - (x_1, \ldots, x_n)$ belongs to the null space of D_{b^*}. Hence, $\gamma - (x_1, \ldots, x_n) + \gamma = 2\gamma - (x_1, \ldots, x_n)$ belongs to D_{b^*}. For $x = 0, \ldots, q-1$,

$$W^{-1}(x) = \begin{cases} x/2, & \text{for even } x; \\ q - (x+1)/2, & \text{for odd } x, \end{cases}$$

and

$$\begin{aligned} W^{-1}(q-1-x) &= \begin{cases} (q-1)/2 - W^{-1}(x), & \text{for even } x; \\ (3q-1)/2 - W^{-1}(x), & \text{for odd } x, \end{cases} \\ &= 2\gamma - W^{-1}(x). \end{aligned}$$

Then $W^{-1}(q-1-W(x_1, \ldots, x_n)) = 2\gamma - (x_1, \ldots, x_n)$. Hence, $W^{-1}(q-1-W(x_1, \ldots, x_n))$ belongs to D_{b^*}. This completes the proof. □

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