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OPTIMAL MAXIMIN L_1-DISTANCE LATIN HYPERCUBE DESIGNS BASED ON GOOD LATTICE POINT DESIGNS[1]

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Maximin distance Latin hypercube designs are commonly used for computer experiments, but the construction of such designs is challenging. We construct a series of maximin Latin hypercube designs via Williams transformations of good lattice point designs. Some constructed designs are optimal under the maximin L_1-distance criterion, while others are asymptotically optimal. Moreover, these designs are also shown to have small pairwise correlations between columns.

1. Introduction. Computer experiments are increasingly being used to investigate complex systems [Sacks, Schiller and Welch (1989), Santner, Williams and Notz (2003), Fang, Li and Sudjianto (2006), Morris and Moore (2015)]. A general design approach to planning computer experiments is to seek design points that fill a design region as uniformly as possible [Lin and Tang (2015)]. Representative designs include Latin hypercube designs (LHDs) and their modifications, maximin distance designs [Johnson, Moore and Ylvisaker (1990)] and uniform designs [Fang and Wang (1994)]. LHDs have uniform one-dimensional projections and orthogonal-array based LHDs [Tang (1993), He and Tang (2013, 2014), He, Cheng and Tang (2018)] have improved two- or three-dimensional projections. Many researchers have constructed orthogonal or nearly orthogonal LHDs; see, among others, Ye (1998), Steinberg and Lin (2006), Cioppa and Lucas (2007), Lin, Mukerjee and Tang (2009), Sun, Liu and Lin (2009), Yang and Liu (2012), Georgiou and Efthimiou (2014), Lin and Tang (2015) and Sun and Tang (2017). However, these LHDs are often not space-filling in high dimensions [Joseph and Hung (2008), Xiao and Xu (2018)].

A maximin distance design spreads design points over the design space in such a way that the separation distance, that is, the minimal distance between pairs of points, is maximized. Computer experiments are often modeled as Gaussian processes. When the correlations between observations rapidly decrease as the distances between design points increase, maximin distance designs are asymptotically D-optimal in the sense that they maximize the determinant of the correlation matrix [Johnson, Moore and Ylvisaker (1990)]. The choice of distances is

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application dependent. Some researchers worked on the L_2-distance and proposed algorithms such as simulated annealing [Morris and Mitchell (1995), Joseph and Hung (2008), Ba, Myers and Brenneman (2015)] and swarm optimization algorithms [Moon, Dean and Santner (2011), Chen et al. (2013)] to construct maximin distance LHDs. However, such methods are not efficient for constructing large designs due to their computational complexity. Nevertheless, large designs are needed for computer experiments; for example, Morris (1991) considered many simulation models involving hundreds of factors. Zhou and Xu (2015) studied both L_1- and L_2-distances of good lattice point (GLP) designs. The GLP method was introduced by Korobov (1959) for numerical evaluation of multivariate integrals and has been widely used in quasi-Monte Carlo method, uniform designs and computer experiments [Fang and Wang (1994)]. Zhou and Xu (2015) showed that permuting levels can increase the separation distances of GLP designs. It is infeasible to conduct all level permutations, so they considered only linear permutations, which limits the ability of generating good designs. Xiao and Xu (2017) proposed construction methods via Costas' arrays and obtained some LHDs with large minimal L_1-distance.

In this paper, we propose a series of systematic methods to construct maximin L_1-distance LHDs. The L_1-distance provides a lower bound for the L_2-distance by the Cauchy–Schwarz inequality so that the constructed designs also perform well regarding the L_2-distance. The proposed method is based on the Williams transformation and its modification. The Williams transformation was first used by Williams (1949) to construct Latin square designs that are balanced for nearest neighbors. Bailey (1982) and Edmondson (1993) used the transformation to construct designs orthogonal to polynomial trends. Butler (2001) used the transformation to construct optimal and orthogonal LHDs under a second-order cosine model. Our purpose is different from theirs. We apply the Williams transformation to GLP designs and construct a class of asymptotically optimal maximin LHDs. Applying the leave-one-out method we obtain another class of asymptotically optimal maximin LHDs. By modifying the Williams transformation, we obtain a class of exactly optimal maximin LHDs. Moreover, all resulting designs have small pairwise correlations between columns and the average correlations converge to zero as the design sizes increase. This near orthogonality is desirable for estimating potential linear trend efficiently in a Gaussian process.

This paper is organized as follows. Section 2 provides the construction methods. Sections 3 and 4 give theoretical results on separation distances and correlations of some special constructed designs. Section 5 extends the theoretical results to a general situation. Concluding remarks are given in Section 6. Proofs are deferred to the Appendix.

2. Construction methods. An $N \times n$ LHD is an $N \times n$ matrix where each column is a permutation of N equally spaced levels, denoted by $0, \dots, N-1$ or $1, \dots, N$. The L_1-distance between two vectors $x_1 = (x_{11}, \dots, x_{1n})$ and $x_2 =$

$(x_{21}, \dots, x_{2n})$ is $d(x_1, x_2) = \sum_{j=1}^{n} |x_{1j} - x_{2j}|$. For an $N \times n$ design matrix D, let x_i be the ith row, $i = 1, \dots, N$, and $d_{ik}(D)$ be the L_1-distance between the ith and kth rows of D, that is, $d_{ik}(D) = d(x_i, x_k)$. The L_1-distance of D, denoted by $d(D) = \min\{d_{ik}(D) : i \neq k,\ i, k = 1, \dots, N\}$, is the minimum L_1-distance between any two distinct rows in D. The maximin distance criterion [Johnson, Moore and Ylvisaker (1990)] is to maximize $d(D)$ among all possible designs. For an $N \times n$ LHD, the average pairwise L_1-distance between rows is $(N + 1)n/3$ [Zhou and Xu (2015)]. Because the minimum pairwise L_1-distance cannot exceed the integer part of the average, we have the following result.

LEMMA 1. *For any $N \times n$ LHD D, $d(D) \leq d_{\text{upper}} = \lfloor (N + 1)n/3 \rfloor$, where $\lfloor x \rfloor$ is the integer part of x.*

Let $h = (h_1, \dots, h_n)$ be a set of positive integers smaller than and coprime to N. An $N \times n$ GLP design $D = (x_{ij})$ is defined by $x_{ij} = i \times h_j \pmod N$ for $i = 1, \dots, N$ and $j = 1, \dots, n$. The last row of D is a vector of zeros. Each column of D is a permutation of $\{0, \dots, N - 1\}$. Thus a GLP design is an LHD. We can construct an $N \times n$ GLP design for any $n \leq \phi(N)$, where $\phi(N)$ is the Euler function, that is, the number of positive integers smaller than and coprime to N. Let $D_b = D + b \pmod N$ for $b = 0, \dots, N - 1$, that is, D_b is a linearly permuted GLP design. Then D_b is still an LHD. Zhou and Xu (2015) showed that $d(D_b) \geq d(D)$ for any b and proposed to search b that maximizes $d(D_b)$.

2.1. *Williams' transformation*. Given an integer N, for $x = 0, \dots, N - 1$, the Williams transformation is defined by

$$W(x) = \begin{cases} 2x & \text{for } 0 \leq x < N/2; \\ 2(N - x) - 1 & \text{for } N/2 \leq x < N. \end{cases} \tag{2.1}$$

The Williams transformation is a permutation of $\{0, \dots, N - 1\}$. Hence, for an LHD $D = (x_{ij})$, $W(D) = (W(x_{ij}))$ is also an LHD. The following example shows that the Williams transformation can further increase the L_1-distance of linearly permuted GLP designs.

EXAMPLE 1. Consider $N = 11$ and $h = (1, \dots, 10)$. The GLP design $D = (x_{ij})$ is an 11×10 LHD with $x_{ij} = i \times j \pmod{11}$ and $d(D) = 30$. For each $b = 0, \dots, 10$, we obtain two designs via linear permutation and Williams' transformation, namely, $D_b = D + b \pmod{11}$ and $E_b = W(D_b)$. Table 1 shows the L_1-distances of D_b and E_b. The linearly permuted designs D_b's have distances ranging from 30 to 34, while the distances for E_b's vary from 10 to 39. The upper bound from Lemma 1 is 40. The best design from D_b's is D_1 or D_9 with $d(D_1) = d(D_9) = 34$, while the best design from E_b's is E_1 or E_4 with $d(E_1) = d(E_4) = 39$.

TABLE 1
The L_1-distances of D_b and E_b in Example 1

b	0	1	2	3	4	5	6	7	8	9	10
$d(D_b)$	30	34	30	32	31	30	31	32	30	34	30
$d(E_b)$	10	39	31	31	39	10	28	34	30	34	28

Example 1 shows that the Williams transformation can generate designs with larger distances than the linear permutation. Inspired by this, we propose a new construction for maximin LHDs:

ALGORITHM 1 (Williams' transformation of linearly permuted GLP designs).

Step 1. Given a pair of integers N and $n \le \phi(N)$, generate an $N \times n$ GLP design D.

Step 2. For $b = 0, \dots, N-1$, generate $D_b = D + b \pmod N$ and $E_b = W(D_b)$.

Step 3. Find the best D_b and E_b which maximize $d(D_b)$ and $d(E_b)$, respectively.

As an illustration, we apply Algorithm 1 for $N = 7, \dots, 30$ and $n = \phi(N)$. Table 2 compares LHDs generated by the linear permutation, the Williams transformation, R package SLHD provided by Ba, Myers and Brenneman (2015) and the Gilbert and Golomb methods proposed by Xiao and Xu (2017). The SLHD package adopts the L_2-distance measure, so we ran the command `maximinSLHD` with option $t = 1$ and default settings for 100 times, and chose the design with the largest L_1-distance. The Williams transformation always offers better designs than the linear permutation except for $N = 13$, and consistently outperforms the Gilbert and Golomb methods, which only work for prime N. Compared to the SLHD package, the Williams transformation performs better for designs with moderate to large sizes. The Williams transformation performs specially well when N is a prime.

2.2. *Leave-one-out method.* Since the last row of a GLP design D is $(0, \dots, 0)$, then the last rows of D_b and E_b are $(b, \dots, b)$ and $(W(b), \dots, W(b))$, respectively. The leave-one-out method is to delete the constant row of a design and rearrange the levels so that the resulting design is still an LHD. Specifically, starting from D_b, we delete the last row and reduce the levels $b+1, \dots, N-1$ by one, which gives us an $(N-1) \times n$ LHD, denoted by D_b^*. Similarly, from E_b, we obtain another $(N-1) \times n$ LHD, denoted by E_b^*. Table 3 compares the

TABLE 2
Comparison of L_1-distances of $N \times n$ LHDs

N	**n**	**LP**	**WT**	**SLHD**	**Gil**	**Gol**	**N**	**n**	**LP**	**WT**	**SLHD**	**Gil**	**Gol**
7	6	13	16	15	14	14	19	18	106	115	108	102	106
8	4	8	10	11			20	8	32	42	43		
9	6	15	16	18			21	12	66	76	73		
10	4	8	11	11			22	10	60	68	61		
11	10	34	39	36	34	34	23	22	154	168	160	154	158
12	4	8	10	13			24	8	32	36	50		
13	12	54	52	52	46	48	25	20	147	162	153		
14	6	22	24	23			26	12	84	98	87		
15	8	29	36	35			27	18	135	156	145		
16	8	32	36	37			28	12	72	94	92		
17	16	84	94	86	86	80	29	28	250	274	254	250	244
18	6	18	28	28			30	8	40	62	57		

Note: LP, linear permutation; WT, Williams' transformation; SLHD, R package SLHD; Gil, Gilbert method; Gol, Golomb method.

L_1-distances of D_b^* and E_b^* for $N = 7, \dots, 30$, as well as the $(N-1) \times n$ designs generated by R package SLHD and the Gilbert and Golomb methods. From Table 3,the leave-one-out Williams transformation generates designs with larger L_1-distance than other methods in most cases. It performs specially well when N is a prime.

TABLE 3
Comparison of L_1-distances of $(N-1) \times n$ LHDs

N	**n**	**LP-1**	**WT-1**	**SLHD**	**Gil**	**Gol**	**N**	**n**	**LP-1**	**WT-1**	**SLHD**	**Gil**	**Gol**
7	6	12	14	14	14	14	19	18	104	112	103	102	106
8	4	8	9	9			20	8	37	40	41		
9	6	14	14	16			21	12	64	74	71		
10	4	10	10	11			22	10	56	64	60		
11	10	34	36	34	34	34	23	22	152	166	152	154	158
12	4	8	10	12			24	8	32	36	47		
13	12	52	50	47	46	48	25	20	146	156	146		
14	6	19	23	22			26	12	80	93	85		
15	8	28	34	34			27	18	134	152	139		
16	8	32	34	36			28	12	81	91	89		
17	16	82	88	82	86	80	29	28	244	268	247	250	244
18	6	18	27	26			30	8	40	60	56		

Note: LP-1, leave-one-out linear permutation; WT-1, leave-one-out Williams transformation.

2.3. *Modified Williams' transformation.* To construct other maximin LHDs, we propose a modified Williams transformation. For $x = 0, \dots, N-1$, define

$$w(x) = \begin{cases} 2x & \text{for } 0 \le x < N/2; \\ 2(N-x) & \text{for } N/2 \le x < N. \end{cases} \tag{2.2}$$

The following lemma shows an important connection between the original and modified Williams transformations.

LEMMA 2. *Let N be an odd prime, D be an $N \times (N-1)$ GLP design and $D_b = D + b \pmod N$ for $b = 0, \dots, N-1$. Then $d_{ik}(w(D_b)) = d_{ik}(W(D_b))$ for $i + k \neq N$ and $i, k = 1, \dots, N-1$.*

The $w(x)$ is always an even number, so $w(D_b)$ is not an LHD. We can construct LHDs by selecting some submatrices of $w(D)/2$. Let us see an illustrating example.

EXAMPLE 2. Consider $N = 11$ and the 11×10 GLP design D. The design matrices of D and $w(D)/2$ are shown in Table 4. If we divide the design matrix of $w(D)/2$ into four blocks as shown in Table 4, then each block is a LHD. Denote H_1 and H_2 as the top two blocks, and H_3 and H_4 as the bottom two blocks, respectively. It can be verified that H_1 and H_2 are 5×5 LHDs with $d(H_1) = d(H_2) = 10$, which attains the upper bound of L_1-distance in Lemma 1. In fact, H_1 and H_2 are the same design up to column permutations; in addition, H_3 and H_4 can be obtained by adding a row of zeros to H_1 and H_2, respectively.

Generally, suppose that N is an odd prime with $N = 2m + 1$ and $D = (x_{ij})$ is the $N \times (N-1)$ GLP design. Since $x_{ij} + x_{(N-i)j} = N$ and $x_{ij} + x_{i(N-j)} = N$ for

TABLE 4
The design matrices of D and $w(D)/2$ in Example 2

D										**w(D)/2**									
1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	5	4	3	2	1
2	4	6	8	10	1	3	5	7	9	2	4	5	3	1	1	3	5	4	2
3	6	9	1	4	7	10	2	5	8	3	5	2	1	4	4	1	2	5	3
4	8	1	5	9	2	6	10	3	7	4	3	1	5	2	2	5	1	3	4
5	10	4	9	3	8	2	7	1	6	5	1	4	2	3	3	2	4	1	5
6	1	7	2	8	3	9	4	10	5	5	1	4	2	3	3	2	4	1	5
7	3	10	6	2	9	5	1	8	4	4	3	1	5	2	2	5	1	3	4
8	5	2	10	7	4	1	9	6	3	3	5	2	1	4	4	1	2	5	3
9	7	5	3	1	10	8	6	4	2	2	4	5	3	1	1	3	5	4	2
10	9	8	7	6	5	4	3	2	1	1	2	3	4	5	5	4	3	2	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

TABLE 5
Comparison of L_1-distances of $m \times m$ LHDs

m	MWT	SLHD	Wel	Gil	Gol	*m*	MWT	SLHD	Wel	Gil	Gol
5	10	10	10	10	8	23	184	167	166	164	
6	14	14	12	14	14	26	234	212			
8	24	22				29	290	263	264	266	270
9	30	28			26	30	310	281	240	276	292
11	44	40	40	40	40	33	374	340			
14	70	64				35	420	383			386
15	80	72			72	36	444	402	342	408	404
18	114	103	90	102	106	39	520	473			482
20	140	126				41	574	523	524	534	520
21	154	141			140	44	660	604			

Note: MWT, modified Williams' transformation; Wel, Welch.

any $i, j = 1, \dots, N-1$, then

$$D = \begin{pmatrix} A_1 & N - A_2 \\ N - A_3 & A_4 \\ 0_m & 0_m \end{pmatrix} \quad \text{and} \quad w(D) = \begin{pmatrix} w(A_1) & w(A_2) \\ w(A_3) & w(A_4) \\ 0_m & 0_m \end{pmatrix}, \tag{2.3}$$

where A_1 is the $m \times m$ leading principal submatrix of D, and A_2, A_3 and A_4 can be obtained from A_1 by reversing the order of columns, rows and both, respectively. In fact, $w(A_1), \dots, w(A_4)$ are the same design up to row and column permutations, each column of which is a permutation of $\{2, 4, \dots, 2m\}$. Let

$$H = w(A_1)/2 \tag{2.4}$$

be an $m \times m$ LHD from the modified Williams transformation. Table 5 compares LHDs generated by the modified Williams transformation, the R package SLHD and the Welch, Gilbert and Golomb methods from Xiao and Xu (2017). The modified Williams transformation always provides better designs than any other methods. In fact, the L_1-distance of each design generated by the modified Williams transformation in Table 5 attains the upper bound given in Lemma 1.

3. Theoretical results. The Williams transformation leads to a remarkably simple design structure in terms of the L_1-distance when N is an odd prime.

THEOREM 1. *Let N be an odd prime, D be an $N \times (N-1)$ GLP design, $D_b = D + b \pmod N$ and $E_b = W(D_b)$ for $b = 0, \dots, N-1$. Then for $i \neq k$,*

$$d_{ik}(E_b) = \begin{cases} (N^2-1)/3 + f(b) & \text{for } i = N \text{ or } k = N, \\ (N^2-1)/3 - 2f(b) & \text{for } i = N - k, \\ (N^2-1)/3 & \text{otherwise,} \end{cases}$$

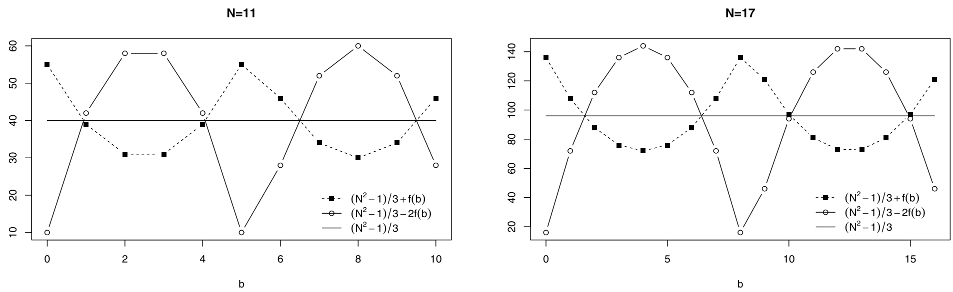

FIG. 1. *The three possible values of pairwise L_1-distance of E_b for $N = 11$ or 17.*

and $d(E_b) = (N^2 - 1)/3 + \min\{f(b), -2f(b)\}$, *where* $f(b) = (W(b) - (N - 1)/2)^2 - (N^2 - 1)/12$.

The pairwise L_1-distance between any two distinct rows of E_b takes on only three possible values. One attains $d_{\text{upper}} = (N^2 - 1)/3$ given in Lemma 1, and the other two vary around d_{upper}. Figure 1 shows the three values for $N = 11$ and $N = 17$ for each $b = 0, \dots, N - 1$.

To maximize $d(E_b)$, we need to maximize $\min\{f(b), -2f(b)\}$. Let $c_0 = \lfloor\sqrt{(N^2 - 1)/12}\rfloor$,

$$c = \begin{cases} c_0 & \text{if } c_0^2 + 2(c_0 + 1)^2 \geq (N^2 - 1)/4; \\ c_0 + 1 & \text{otherwise,} \end{cases}$$

and

$$b = W^{-1}\left(\frac{N - 1}{2} \pm c\right). \tag{3.1}$$

It can be verified that either choice of b defined in (3.1) maximizes $\min\{f(b), -2f(b)\}$ and leads to the best E_b.

EXAMPLE 3. Consider $N = 11$. Then $c_0 = \lfloor\sqrt{(11^2 - 1)/12}\rfloor = 3$. Since $c_0^2 + 2(c_0 + 1)^2 \geq (N^2 - 1)/4$, set $c = 3$. By (3.1), $b = 1$ or 4. For either $b = 1$ or $b = 4$, by Theorem 1, for $i \neq k$,

$$d_{ik}(E_b) = \begin{cases} 39 & \text{for } i = 11 \text{ or } k = 11, \\ 42 & \text{for } i = 11 - k, \\ 40 & \text{otherwise.} \end{cases}$$

Hence, $d(E_1) = d(E_4) = 39$.

Based on the upper bound in Lemma 1, we define the distance efficiency as

$$d_{\text{eff}}(D) = d(D)/d_{\text{upper}} = d(D)/\lfloor(N + 1)n/3\rfloor. \tag{3.2}$$

When N is a prime, $n = \phi(N) = N - 1$ and $(N+1)n/3 = (N^2-1)/3$ is an integer. In this case, $d_{\text{eff}}(D) = d(D)/((N+1)n/3)$. For example, for the designs E_1 and E_4 in Example 3, $d_{\text{eff}}(E_1) = d_{\text{eff}}(E_4) = 39/40 = 0.975$. Generally, we have the following result.

THEOREM 2. *For an odd prime N and b defined in* (3.1),

$$d(E_b) \geq \frac{N^2-1}{3} - \frac{2}{3}\sqrt{\frac{N^2-1}{3}} \quad \text{and} \quad d_{\text{eff}}(E_b) \geq 1 - \frac{2}{\sqrt{3(N^2-1)}}.$$

As $N \to \infty$, $d_{\text{eff}}(E_b) \to 1$; so E_b is asymptotically optimal under the maximin distance criterion. For the leave-one-out design E_b^* defined in Section 2.2, we have the following result.

THEOREM 3. *For an odd prime N and b defined in* (3.1),

$$d(E_b^*) \geq \frac{N^2-7}{3} + \frac{1}{3}\sqrt{\frac{N^2-1}{3}} - (N-1).$$

When $N \geq 7$, $d_{\text{eff}}(E_b^*) \geq 1 - (3 - 1/\sqrt{3})/N > 1 - 2.43/N$.

For an odd prime $N = 2m+1$ and the $m \times m$ design H constructed in (2.4), we have even better results. By Lemma 2 and Theorem 1, $d_{ik}(w(D)) = (N^2-1)/3$ for $i \neq k$, $i, k = 1, \dots, m$. By the structure of $w(D)$ shown in (2.3), $d_{ik}(w(A_1)) = d_{ik}(w(D))/2 = (N^2-1)/6$; so H is an equidistant LHD and $d(H) = (N^2-1)/12 = (m+1)m/3$.

THEOREM 4. *Let $N = 2m+1$ be an odd prime, $D = (x_{ij})$ be an $N \times (N-1)$ GLP design, and A_1 be the $m \times m$ leading principal submatrix of D, that is, $A_1 = (x_{ij})$ with $i, j = 1, \dots, m$. Then $H = w(A_1)/2$ is a maximin distance LHD with $d(H) = (m+1)m/3$.*

The modified Williams transformation generates exact maximin LHDs when N is an odd prime. The constructed H is a cyclic Latin square, with each level occurring once in each row and once in each column. We can add a row of zeros to H to obtain an $(m+1) \times m$ LHD, denoted by H^*. It is easy to see that $d(H^*) = d(H) = (m+1)m/3$ and $d_{\text{eff}}(H^*) = (m+1)/(m+2) \to 1$ as $m \to \infty$.

The proposed methods are also useful in the construction of maximin L_2-distance designs. An upper bound for the L_2-distance of an $N \times n$ LHD is $d_{\text{upper}}^{(2)} = \sqrt{N(N+1)n/6}$ [Zhou and Xu (2015)]. By the Cauchy–Schwarz inequality, we have $\|x\|_2 \geq \|x\|_1/\sqrt{n}$ for any n-vector x, so $d_{\text{eff}}^{(2)} > \sqrt{2/3}\, d_{\text{eff}}$, where $d_{\text{eff}}^{(2)}$ is the L_2-distance efficiency. Therefore, for an (asymptotically) optimal design under the maximin L_1-distance criterion, its L_2-distance efficiency will tend to be greater than $\sqrt{2/3} > 0.816$. This is a loose lower bound, and yet it illustrates the good performance of our constructed designs regarding the L_2-distance. Numerical calculation shows that our proposed methods are able to produce designs with L_2-distance efficiencies greater than 0.95 for large N.

4. Additional results on correlations. We now consider the pairwise correlation between columns for the constructed designs. For any $N \times n$ design $D = (x_{ij})$, define

$$\rho_{\text{ave}}(D) = \frac{\sum_{j \neq k} |\rho_{jk}|}{n(n-1)}, \tag{4.1}$$

where ρ_{jk} is the correlation between columns j and k of D. The ρ_{ave} in (4.1) is a performance measure on the overall pairwise column correlations for design D. A good design should have a low ρ_{ave} value to reduce correlations between factors and reduce the variance of coefficients estimates.

Consider the ρ_{ave} values for the designs from the Williams transformation. For each prime N, Table 6 compares the ρ_{ave} values of designs from the linear permutation, Williams transformation [with b chosen by (3.1)], Gilbert and Golomb methods. The Williams transformation always generates designs with the smallest ρ_{ave} values. In fact, we have a general result on the average correlation $\rho_{\text{ave}}(E_b)$ for any $b = 0, \dots, N-1$, not restricted to the b defined in (3.1).

THEOREM 5. *Let N be an odd prime and D be an $N \times (N-1)$ GLP design, $D_b = D + b \pmod N$, and $E_b = W(D_b)$ for $b = 0, \dots, N-1$. Then $\rho_{\text{ave}}(E_b) < 2/(N-2)$.*

For a prime N, $\rho_{\text{ave}}(E_b) \to 0$ as $N \to \infty$ for any $b = 0, \dots, N-1$. This property makes it possible to generate large LHDs with tiny pairwise column correla-

TABLE 6
Comparison of the ρ_{ave} values for $N \times (N-1)$ LHDs

N	LP	WT	Gil	Gol	N	LP	WT	Gil	Gol
7	0.25	0.086	0.25	0.25	47	0.09	0.015	0.09	0.11
11	0.16	0.054	0.19	0.17	53	0.08	0.014	0.07	0.07
13	0.07	0.065	0.16	0.18	59	0.08	0.013	0.08	0.07
17	0.17	0.043	0.13	0.15	61	0.07	0.012	0.07	0.07
19	0.16	0.027	0.18	0.13	67	0.06	0.011	0.08	0.06
23	0.14	0.022	0.12	0.09	71	0.06	0.010	0.07	0.07
29	0.12	0.023	0.11	0.12	73	0.06	0.011	0.06	0.08
31	0.10	0.024	0.09	0.09	79	0.06	0.010	0.06	0.08
37	0.11	0.017	0.10	0.10	83	0.06	0.010	0.06	0.07
41	0.11	0.019	0.11	0.09	89	0.06	0.009	0.07	0.06
43	0.09	0.017	0.09	0.11	97	0.06	0.008	0.07	0.06

TABLE 7
Comparison of the ρ_{ave} values for $(N-1)\times(N-1)$ LHDs

N	**LP-1**	**WT-1**	**Gil**	**Gol**	N	**LP**	**WT-1**	**Gil**	**Gol**
7	0.35	0.211	0.21	0.20	47	0.09	0.029	0.08	0.10
11	0.18	0.121	0.15	0.16	53	0.07	0.027	0.06	0.06
13	0.09	0.140	0.17	0.18	59	0.08	0.026	0.07	0.07
17	0.14	0.095	0.11	0.14	61	0.07	0.023	0.06	0.07
19	0.12	0.063	0.15	0.10	67	0.06	0.022	0.08	0.06
23	0.12	0.050	0.11	0.07	71	0.06	0.020	0.07	0.06
29	0.11	0.046	0.09	0.13	73	0.06	0.021	0.06	0.08
31	0.11	0.049	0.11	0.07	79	0.07	0.020	0.06	0.08
37	0.10	0.034	0.08	0.10	83	0.07	0.019	0.05	0.07
41	0.09	0.038	0.09	0.09	89	0.07	0.018	0.06	0.06
43	0.09	0.032	0.09	0.11	97	0.06	0.016	0.07	0.06

tions without any computer search. For the leave-one-out Williams transformation, we have the following result.

THEOREM 6. *Let N be an odd prime, D be an $N\times(N-1)$ GLP design, $D_b = D + b \pmod N$, $E_b = W(D_b)$, and E_b^* be the leave-one-out design obtained from E_b for $b = 0,\dots,N-1$. Then $\rho_{\text{ave}}(E_b^*) < 5(N+1)/(N-2)^2$ for any $b = 0,\dots,N-1$.*

Table 7 compares designs obtained from the leave-one-out linear permutation, leave-one-out Williams transformation, Gilbert and Golomb methods. The leave-one-out Williams transformation generates designs with the smallest ρ_{ave} values except for $N = 13$.

For the modified Williams transformation, we have the following result.

THEOREM 7. *Let $N = 2m+1$ be an odd prime, $D = (x_{ij})$ be an $N\times(N-1)$ GLP design, A_1 be the $m\times m$ leading principal submatrix of D, that is, $A_1 = (x_{ij})$ with $i, j = 1,\dots,m$, and $H = w(A_1)/2$. Then $\rho_{\text{ave}}(H) < 2/(m-1)$.*

Table 8 compares the ρ_{ave} values of designs generated by the modified Williams transformation and some other available methods. The modified Williams transformation always provides designs with the smallest ρ_{ave} values.

5. Extension. We consider extending the results to a general case where $N = kp$ with k and p being prime numbers. Let

$$b = \lfloor N(1 + 1/\sqrt{3})/4 \rfloor, \tag{5.1}$$

and E_b be the $N\times\phi(N)$ design constructed by the Williams transformation. Figure 2 (top) shows the values of $d_{\text{eff}}(E_b)$ for $N = 2p, 3p, 5p$ and $7p$ and $p \le 200$.

TABLE 8
Comparison of the ρ_{ave} values for $m \times m$ LHDs

m	MWT	Wel	Gil	Gol	*m*	MWT	Wel	Gil	Gol
5	0.250	0.25	0.25	0.45	23	0.055	0.12	0.14	
6	0.200	0.29	0.21	0.20	26	0.049			
8	0.143				29	0.045	0.11	0.09	0.08
9	0.125			0.20	30	0.044	0.11	0.11	0.07
11	0.100	0.17	0.14	0.15	33	0.040			
14	0.080				35	0.038			0.09
15	0.077			0.17	36	0.037	0.13	0.08	0.10
18	0.067	0.17	0.15	0.10	39	0.035			0.09
20	0.061				41	0.033	0.11	0.11	0.11
21	0.059			0.11	44	0.031			

The $d_{\text{eff}}(E_b)$ increases quickly as N increases and reaches 0.9 when N is around 30. When $N > 100$, the $d_{\text{eff}}(E_b)$ values are typically greater than 0.95 and converge to 1 for $N = 2p$ and $N = 7p$. The $d_{\text{eff}}(E_b)$ values do not converge to 1 for $N = 3p$ and $N = 5p$, possibly due to the looseness of the upper bound d_{upper}. In addition, Figure 2 (bottom) shows that $\rho_{\text{ave}}(E_b)$ goes to 0 quickly as N increases.

We present the asymptotic optimality of E_b for $N = 2p$ based on the theoretical results in Section 3. It is possible to establish similar results for other cases with more elaborate arguments, which we do not pursue here.

THEOREM 8. *Let p be an odd prime, $N = 2p$, D be an $N \times \phi(N)$ GLP design, $D_b = D + b \pmod N$ and $E_b = W(D_b)$. For b defined in* (5.1), $d_{\text{eff}}(E_b) = 1 - O(1/N)$. *As $N \to \infty$, $d_{\text{eff}}(E_b) \to 1$.*

Now we consider an extension of the leave-one-out procedure. We can generate many asymptotically optimal LHDs by applying the following leave-out-one procedure for rows or columns. When we delete any row from an $N \times n$ LHD D and rearrange the levels as in the leave-one-out method in Section 2.2, the distance of the resulting design will reduce at most by n. When we delete any column from an $N \times n$ LHD D, the distance will reduce at most by $N - 1$. Deleting multiple columns and rows together is equivalent to repeating the leave-one-out procedure for multiple times. The following result can be derived.

THEOREM 9. *Let D be an $N \times n$ LHD. Deleting any k_r rows and k_c columns and rearranging the levels yields an $(N - k_r) \times (n - k_c)$ LHD, denoted by D^*. Then $d_{\text{eff}}(D^*) \geq d_{\text{eff}}(D) - 3k_r/(N - k_r) - 3k_c/(n - k_c)$.*

For $N = kp$ and $n = \phi(N)$, $n \to \infty$ as $N \to \infty$. If k_r and k_c are fixed constants not increasing with N, $d_{\text{eff}}(D^*) \to 1$ as $N \to \infty$. This multiple leave-one-out pro-

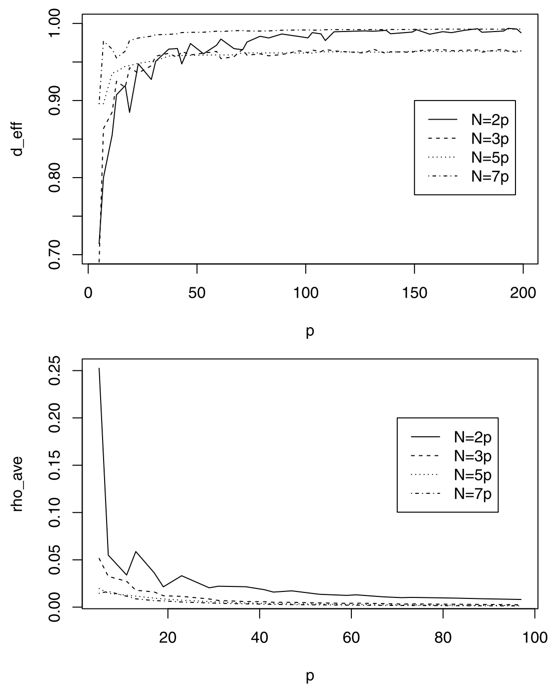

FIG. 2. *The values of* $d_{\text{eff}}(E_b)$ (*top*) *and* $\rho_{\text{ave}}(E_b)$ (*bottom*) *with* b *defined in* (5.1).

cedure yields many asymptotically optimal LHDs with different sizes. For example, let $k = 3$ and $p = 41$, we obtain a 123×80 LHD with $d_{\text{eff}} = 0.956$. Delete the last 22 rows and rearrange the levels; we obtain a 101×80 LHD with $d_{\text{eff}} = 0.948$. Let $k = 2$ and $p = 61$, we obtain a 122×60 LHD with $d_{\text{eff}} = 0.980$. Delete the last 21 rows and rearrange the levels; we obtain a 101×60 LHD with $d_{\text{eff}} = 0.961$. Let $k = 5$ and $p = 103$, we obtain a 515×408 LHD with $d_{\text{eff}} = 0.962$. Delete the last 3 rows and the last 8 columns, and rearrange the levels, we obtain a 512×400 LHD with $d_{\text{eff}} = 0.953$. A distinctive feature of our method is the excellent performance for moderate and large designs. Many other methods slow down quickly as the design size increases and usually give designs with poor distance efficiencies. In contrast, our method generates moderate and large designs with guaranteed high distance efficiencies without search, as long as the ratios of k_r/N and $k_c/\phi(N)$ are small. When the ratios are relatively large, this simple procedure may not work well and further research is needed.

6. Concluding remarks. We have proposed a series of systematic methods for the construction of maximin LHDs via the Williams transformation and its modification. The Williams transformation and leave-one-out method produce asymptotically optimal LHDs under the maximin distance criterion, and the modified Williams transformation generates equidistant LHDs under the L_1-distance.

Xu (1999) showed that equidistant LHDs are universally optimal for computer experiments. The average correlations between columns of the constructed designs converge to zero as the design sizes increase. Moreover, the constructed designs often have larger L_1-distance and smaller average correlation than existing designs even for designs with small sizes.

The Williams transformation can be applied to other designs as well. We have explored the Williams transformation on regular fractional factorial designs and found that it can substantially improve design efficiencies for estimating polynomial models. We will report the results in a separate paper.

APPENDIX: PROOFS

We need to distinguish two addition operations. To clarify, let $\oplus$ be the addition operation over the Galois field $\{0, \ldots, N-1\}$. Let $D = (x_{ij})$ be the $N \times \phi(N)$ GLP design and $D_b = (x_{ij} \oplus b)$. When N is a prime, $x_i = (x_{i1}, \ldots, x_{i(N-1)})$ and $x_i \oplus b = (x_{i1} \oplus b, \ldots, x_{i(N-1)} \oplus b)$ are the ith row of D and D_b, respectively, x_i is a permutation of $\{1, \ldots, N-1\}$ for $i = 2, \ldots, N-1$; and $x_1 = (1, \ldots, N-1)$. The designs D and D_b have some important properties which are crucial for the proofs of all theoretical results. We first summarize these properties in the following lemma.

LEMMA 3. *Let N be an odd prime*:

(i) *For $i \neq k$ and $i, k = 1, \ldots, N-1$, there exists a unique $q \in \{2, \ldots, N-1\}$ such that $k = iq \pmod N$. For any given b, the two matrices*

$$\begin{pmatrix} x_i \oplus b \\ x_k \oplus b \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} x_1 \oplus b \\ x_q \oplus b \end{pmatrix}$$

are the same up to column permutations. In addition, $q = N-1$ if and only if $i + k = N$.

(ii) *For any $b = 0, \ldots, N-1$ and $i = 2, \ldots, N-2$, denote $a = (1-i)b \pmod N$. The two matrices*

$$\begin{pmatrix} x_1 \oplus b & b \\ x_i \oplus b & b \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} x_1 & 0 \\ x_i \oplus a & a \end{pmatrix}$$

are the same up to column permutations.

PROOF. Part (i) is obvious from the definition of D and D_b. For (ii), denote $\tilde{x}_i = (x_i, 0)$ for $i = 1, \ldots, N$. Then $\tilde{x}_i \oplus b = i(\tilde{x}_1 \oplus b) \oplus a$. The result follows by noting that $\tilde{x}_1 \oplus b$ is a permutation of $\tilde{x}_1$ and $i\tilde{x}_1 \oplus a = \tilde{x}_i \oplus a = (x_i \oplus a, a)$. $\square$

PROOF OF LEMMA 2. We divide the proof in four steps.

Step 1. For $i + k \neq N$, $i \neq k$, and $i, k = 1, \ldots, N-1$, by Lemma 3(i), there exists a unique $q \in \{2, \ldots, N-2\}$ such that $d_{ik}(W(D_b)) = d_{1q}(W(D_b))$ and

$d_{ik}(w(D_b)) = d_{1q}(w(D_b))$. Therefore, it suffices to show that $d_{1i}(W(D_b)) = d_{1i}(w(D_b))$ for any $b = 0, \dots, N-1$ and $i = 2, \dots, N-2$.

Step 2. By Lemma 3(ii), to prove $d_{1i}(W(D_b)) = d_{1i}(w(D_b))$, we only need to show that $d(W(x_1), W(x_i \oplus a)) + W(a) = d(w(x_1), w(x_i \oplus a)) + w(a)$ for any $a = 0, \dots, N-1$. Note that $W(a) = w(a)$ if $a < N/2$, and $W(a) = w(a) - 1$ if $a > N/2$. It suffices to show that

$$d\big(W(x_1), W(x_i \oplus a)\big) = \begin{cases} d\big(w(x_1), w(x_i \oplus a)\big) & \text{if } a < N/2; \\ d\big(w(x_1), w(x_i \oplus a)\big) + 1 & \text{if } a > N/2. \end{cases} \tag{A.1}$$

Step 3. Recall that $x_1 = (1, \dots, N-1)$ and $x_i \oplus a = (x_{i1} \oplus a, \dots, x_{i(N-1)} \oplus a)$. Then $d(W(x_1), W(x_i \oplus a)) = \sum_{j=1}^{N-1} |W(j) - W(x_{ij} \oplus a)|$ and $d(w(x_1), w(x_i \oplus a)) = \sum_{j=1}^{N-1} |w(j) - w(x_{ij} \oplus a)|$. It can be shown that

$$\big|W(j) - W(x_{ij} \oplus a)\big| = \begin{cases} \big|w(j) - w(x_{ij} \oplus a)\big| & \text{for } j \in I \cup J; \\ \big|w(j) - w(x_{ij} \oplus a)\big| - 1 & \text{for } j \in U \backslash I; \\ \big|w(j) - w(x_{ij} \oplus a)\big| + 1 & \text{for } j \in V \backslash J, \end{cases}$$

where

$$\begin{aligned} I &= \{j : j < N/2, (x_{ij} \oplus a) < N/2\}, \\ J &= \{j : j > N/2, (x_{ij} \oplus a) > N/2\}, \\ U &= \{j : j + (x_{ij} \oplus a) < N\} \quad \text{and} \quad V = \{j : j + (x_{ij} \oplus a) \geq N\}. \end{aligned}$$

Therefore, to prove (A.1), we need to show that if $a < N/2$, $U \backslash I$ and $V \backslash J$ contain the same number of elements; and if $a > N/2$, $U \backslash I$ contains one less element than $V \backslash J$.

Step 4. Denote $\#S$ as the number of elements in a set S. Since $\#(U \backslash I) = \#U - \#I$ and $\#(V \backslash J) = \#V - \#J$, we want to show that

$$\#U = \#V \quad \text{and} \quad \begin{cases} \#I = \#J & \text{if } a < N/2; \\ \#I = \#J + 1 & \text{if } a > N/2. \end{cases}$$

Since

$$x_{(i+1)j} \oplus a = \begin{cases} j + (x_{ij} \oplus a) & \text{for } j \in U; \\ j + (x_{ij} \oplus a) - N & \text{for } j \in V, \end{cases}$$

then $\sum_{j=1}^{N-1} (x_{(i+1)j} \oplus a) = \sum_{j=1}^{N-1} (x_{ij} \oplus a) + \sum_{j=1}^{N-1} j - (\#V)N$. Because both x_i and x_{i+1} are permutations of $\{1, \dots, N-1\}$, $\sum_{j=1}^{N-1} (x_{(i+1)j} \oplus a) = \sum_{j=1}^{N-1} (x_{ij} \oplus a)$, which leads to $\#V = \sum_{j=1}^{N-1} j/N = (N-1)/2$. Because $\#U + \#V = N - 1$, $\#U = \#V = (N-1)/2$. Denote $I_1 = \{j : j > N/2, (x_{ij} \oplus a) < N/2\}$. If $a < N/2$, $\#I + \#I_1 = \#J + \#I_1 = (N-1)/2$ so $\#I = \#J$. If $a > N/2$, $\#I + \#I_1 = (N+1)/2$ and $\#J + \#I_1 = (N-1)/2$ so $\#I = \#J + 1$. This completes the proof. □

To prove Theorem 1, we need the following lemma.

LEMMA 4. *For all* $i = 2, \dots, N-2$ *and* $b = 0, \dots, N-1$, $d(x_1 \oplus b, x_i \oplus b) + d(N - (x_1 \oplus b), x_i \oplus b) = (2N^2+1)/3 - |N-2b|$.

PROOF. We divide the proofs in three steps.

Step 1. By Lemma 3(ii),

$$d(x_1 \oplus b, x_i \oplus b) = d(x_1, x_i \oplus a) + a$$

and

$$d\big(N - (x_1 \oplus b), x_i \oplus b\big) + |N - 2b| = d(N - x_1, x_i \oplus a) + N - a,$$

where $a = (1-i)b \pmod N$. Then

$$\begin{aligned} &d(x_1 \oplus b, x_i \oplus b) + d\big(N - (x_1 \oplus b), x_i \oplus b\big) \\ &\quad = d(x_1, x_i \oplus a) + d(N - x_1, x_i \oplus a) + N - |N - 2b|. \end{aligned}$$

Hence, it suffices to show that $d(x_1, x_i \oplus a) + d(N - x_1, x_i \oplus a) = (2N^2+1)/3 - N = (N-1)(2N-1)/3$ for any $a = 0, \dots, N-1$.

Step 2. Let $g_i(a) = d(x_1, x_i \oplus a) + d(N - x_1, x_i \oplus a)$. If we can prove $g_i(0) = g_i(1) = \cdots = g_i(N-1)$, we will have

$$g_i(a) = \frac{1}{N} \sum_{c=0}^{N-1} g_i(c) = \frac{1}{N} \sum_{c=0}^{N-1} \big(d(x_1, x_i \oplus c) + d(N - x_1, x_i \oplus c)\big).$$

Because $\sum_{c=0}^{N-1} d(N - x_1, x_i \oplus c) = \sum_{c=0}^{N-1} d(x_1, x_i \oplus c)$, then

$$\begin{aligned} g_i(a) &= \frac{2}{N} \sum_{c=0}^{N-1} d(x_1, x_i \oplus c) = \frac{2}{N} \sum_{c=0}^{N-1} \sum_{j=1}^{N-1} \big|j - (x_{ij} \oplus c)\big| \\ &= \frac{2}{N} \sum_{j=1}^{N-1} \sum_{k=0}^{N-1} |j - k| = (N-1)(2N-1)/3. \end{aligned}$$

Step 3. Now we prove that $g_i(0) = g_i(1) = \cdots = g_i(N-1)$. It suffices to show that $g_i(a+1) = g_i(a)$ for any $a = 0, \dots, N-2$. Recall that $g_i(a) = d(x_1, x_i \oplus a) + d(N - x_1, x_i \oplus a) = \sum_{j=1}^{N-1} (|j - (x_{ij} \oplus a)| + |N - j - (x_{ij} \oplus a)|)$. Since

$$\begin{aligned} &\big|j - \big(x_{ij} \oplus (a+1)\big)\big| + \big|N - j - \big(x_{ij} \oplus (a+1)\big)\big| \\ &\quad = \begin{cases} \big|j - (x_{ij} \oplus a)\big| + \big|N - j - (x_{ij} \oplus a)\big| & \text{for } j \in S_1 \cup S_2; \\ \big|j - (x_{ij} \oplus a)\big| + \big|N - j - (x_{ij} \oplus a)\big| + 2 & \text{for } j \in S_3; \\ \big|j - (x_{ij} \oplus a)\big| + \big|N - j - (x_{ij} \oplus a)\big| - 2 & \text{for } j \in S_4, \end{cases} \end{aligned}$$

where

$$S_1 = \{j : j \le x_{ij} \oplus a < N - j\},$$
$$S_2 = \{j : N - j \le x_{ij} \oplus a < j\},$$
$$S_3 = \{j : x_{ij} \oplus a \ge j, x_{ij} \oplus a \ge N - j\},$$
$$S_4 = \{j : x_{ij} \oplus a < j, x_{ij} \oplus a < N - j\},$$

we only need to show that $\#S_3 = \#S_4$. Note that

$$\begin{cases} x_{(i-1)j} \oplus a = x_{ij} \oplus a - j \\ \quad \text{and } x_{(i+1)j} \oplus a = x_{ij} \oplus a + j & \text{for } j \in S_1; \\ x_{(i-1)j} \oplus a = x_{ij} \oplus a - j + N \\ \quad \text{and } x_{(i+1)j} \oplus a = x_{ij} \oplus a + j - N & \text{for } j \in S_2; \\ x_{(i-1)j} \oplus a = x_{ij} \oplus a - j \\ \quad \text{and } x_{(i+1)j} \oplus a = x_{ij} \oplus a + j - N & \text{for } j \in S_3; \\ x_{(i-1)j} \oplus a = x_{ij} \oplus a - j + N \\ \quad \text{and } x_{(i+1)j} \oplus a = x_{ij} \oplus a + j & \text{for } j \in S_4. \end{cases}$$

Then

$$\text{(A.2)} \quad \sum_{j=1}^{N-1} \big((x_{(i-1)j} \oplus a) + (x_{(i+1)j} \oplus a)\big) = 2 \sum_{j=1}^{N-1} (x_{ij} \oplus a) - N(\#S_3 - \#S_4).$$

Because $x_i \oplus a$ is a permutation of $\{0, \dots, a-1, a+1, \dots, N-1\}$ for any $i < N$, $\sum_{j=1}^{N-1}(x_{(i-1)j} \oplus a) = \sum_{j=1}^{N-1}(x_{ij} \oplus a) = \sum_{j=1}^{N-1}(x_{(i+1)j} \oplus a)$. By (A.2), $N(\#S_3 - \#S_4) = 0$ so $\#S_3 = \#S_4$. This completes the proof. □

PROOF OF THEOREM 1. For the first case, note that $W(x_i \oplus b)$ is a permutation of $\{0, \dots, W(b) - 1, W(b) + 1, \dots, N - 1\}$, and $W(x_N \oplus b)$ is a constant vector with each component equal to $W(b)$, so $d_{iN}(E_b) = d_{Ni}(E_b) = \sum_{j=0}^{N-1} |j - W(b)| = (N^2 - 1)/3 + f(b)$.

To prove the result for the second case, $i = N - k$, it suffices to prove the result for the third case. This is because the total pairwise L_1-distance between distinct rows of $W(D_b)$ is $t = (N-1)\sum_{j_1=0}^{N-1}\sum_{j_2=0}^{N-1} |j_1 - j_2| = N(N-1)^2(N+1)/6$. Out of all the pairs of distinct rows, $N - 1$ pairs belong to the first case with a total distance $t_1 = (N-1)[(N^2-1)/3 + f(b)]$, $(N-1)(N-3)/2$ pairs belong to the third case with a total distance $t_2 = (N^2-1)(N-1)(N-3)/6$, and $(N-1)/2$ pairs belong to the second case. By Lemma 3(i), $d_{i(N-i)}(E_b) = d_{1(N-1)}(E_b)$ for any i. Therefore, $d_{i(N-i)}(E_b) = (t - t_1 - t_2)/[(N-1)/2] = (N^2-1)/3 - 2f(b)$.

Now we prove the result for the last case where $i \ne N - k$, $i \ne N$, and $k \ne N$. By Lemmas 2 and 3(i), it suffices to consider $d_{1i}(E_b) = d(W(x_1 \oplus b), W(x_i \oplus b)) =$

$d(w(x_1 \oplus b), w(x_i \oplus b))$ for $i = 2, \dots, N-2$. Denote

$$B = (B_1|B_2|B_3|B_4) = \left(\begin{matrix} w(x_1 \oplus b) \\ w(x_i \oplus b) \end{matrix} \middle| \begin{matrix} w(x_1 \oplus b) \\ 2N - w(x_i \oplus b) \end{matrix} \middle| \begin{matrix} 2N - w(x_1 \oplus b) \\ w(x_i \oplus b) \end{matrix} \middle| \begin{matrix} 2N - w(x_1 \oplus b) \\ 2N - w(x_i \oplus b) \end{matrix}\right),$$

then $d_{1i}(E_b) = d(B_1)$. By column permutations, B can be rearranged as

$$C = \left(\begin{matrix} 2(x_1 \oplus b) \\ 2(x_i \oplus b) \end{matrix} \middle| \begin{matrix} 2(x_1 \oplus b) \\ 2N - 2(x_i \oplus b) \end{matrix} \middle| \begin{matrix} 2N - 2(x_1 \oplus b) \\ 2(x_i \oplus b) \end{matrix} \middle| \begin{matrix} 2N - 2(x_1 \oplus b) \\ 2N - 2(x_i \oplus b) \end{matrix}\right).$$

By Lemma 4, $d(B) = d(C) = 4((2N^2+1)/3 - |N-2b|)$. Note that $d(B_1) = d(B_4)$ and $d(B_2) = d(B_3)$. For B_2, in both $w(x_1 \oplus b)$ and $w(x_i \oplus b)$, 0 and $w(b)$ appear once and all other even numbers smaller than N appear twice. Then $d(B_2) = \sum_{j=1}^{N-1}(N - w(x_{1j} \oplus b) - w(x_{ij} \oplus b)) = (N^2+1) - 2|N-2b|$. Therefore, $d_{1i}(E_b) = d(B_1) = (d(B) - 2d(B_2))/2 = (N^2-1)/3$. □

PROOF OF THEOREM 2. If $c_0^2 + 2(c_0+1)^2 \geq (N^2-1)/4$, then $c_0 \geq \sqrt{(N^2-1)/12 - 2/9} - 2/3$ and $c_0^2 \geq (N^2-1)/12 - (4/3)\sqrt{(N^2-1)/12}$. Hence, $d(E_b) = (N^2-1)/4 + c_0^2 \geq (N^2-1)/3 - (4/3)\sqrt{(N^2-1)/12}$. Similarly, if $c_0^2 + 2(c_0+1)^2 < (N^2-1)/4$, $c_0 + 1 \leq \sqrt{(N^2-1)/12 - 2/9} + 1/3$, and $(c_0+1)^2 \leq (N^2-1)/12 + (2/3)\sqrt{(N^2-1)/12}$. Then $d(E_b) = (N^2-1)/2 - 2(c_0+1)^2 \geq (N^2-1)/3 - (4/3)\sqrt{(N^2-1)/12}$. Therefore,

$$d(E_b) \geq \frac{N^2-1}{3} - \frac{4}{3}\sqrt{\frac{N^2-1}{12}} = \frac{N^2-1}{3} - \frac{2}{3}\sqrt{\frac{N^2-1}{3}}.$$

By the definition in (3.2), $d_{\text{eff}}(E_b) = d(E_b)/((N^2-1)/3) \geq 1 - 2/\sqrt{3(N^2-1)}$. □

PROOF OF THEOREM 3. Let $e_i = (e_{i1}, \dots, e_{i(N-1)})$ and $e_k = (e_{k1}, \dots, e_{k(N-1)})$ be two distinct rows of E_b for $i, k = 1, \dots, N-1$, and $e_i^* = (e_{i1}^*, \dots, e_{i(N-1)}^*)$ and $e_k^* = (e_{k1}^*, \dots, e_{k(N-1)}^*)$ be the corresponding rows of E_b^*. For $j = 1, \dots, N-1$, if $e_{ij} > W(b) > e_{kj}$ or $e_{kj} > W(b) > e_{ij}$, $|e_{ij}^* - e_{kj}^*| = |e_{ij} - e_{kj}| - 1$; otherwise, $|e_{ij}^* - e_{kj}^*| = |e_{ij} - e_{kj}|$. Since the number of j's such that $e_{ij} > W(b) > e_{kj}$ [or $e_{kj} > W(b) > e_{ij}$] cannot exceed $\min\{W(b), N-1-W(b)\}$, then $d(E_b^*) \geq d(E_b) - 2\min\{W(b), N-1-W(b)\}$. For the b defined in (3.1), $\min\{W(b), N-1-W(b)\} = (N-1)/2 - c$. Then $d(E_b^*) \geq d(E_b) - (N-1) + 2c \geq d(E_b) - (N-1) + 2(\sqrt{(N^2-1)/12} - 1)$. By Theorem 2, $d(E_b^*) \geq (N^2-7)/3 + \sqrt{(N^2-1)/3}/3 - (N-1)$. When $N \geq 7$, we have $d_{\text{eff}}(E_b^*) = d(E_b^*)/\lfloor N(N-1)/3 \rfloor \geq d(E_b^*)/(N(N-1)/3) \geq 1 + 1/(\sqrt{3}N) - 3/N > 1 - 2.43/N$. $\square$

PROOF OF THEOREM 5. Let ρ_{jk} be the correlation between the jth and kth columns of E_b. Denote the jth column of D_b as $\tilde{z}_j \oplus b$ for $j = 1, \dots, N-1$, then $\tilde{z}_j \oplus b = (x_j \oplus b, b)^{\mathrm{T}}$. By Lemma 3(i), there exists a unique $q \in \{2, \dots, N-1\}$ such that $\rho_{jk} = \rho_{1q}$. Thus,

$$\rho_{\text{ave}}(E_b) = \frac{\sum_{j=2}^{N-1} |\rho_{1j}|}{N-2}, \tag{A.3}$$

where

$$\begin{aligned} \rho_{1j} &= \operatorname{cor}\big(W(\tilde{z}_1 \oplus b), W(\tilde{z}_j \oplus b)\big) \\ &= \frac{\sum_{i=1}^{N} (W(x_{i1} \oplus b) - \frac{N-1}{2})(W(x_{ij} \oplus b) - \frac{N-1}{2})}{(N^3 - N)/12}. \end{aligned} \tag{A.4}$$

For $x \in [0, N]$, the Fourier cosine expansion of $x - N/2$ is given by

$$x - \frac{N}{2} = \sum_{u=1}^{\infty} a_u \cos\left(\frac{u\pi x}{N}\right), \tag{A.5}$$

with

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

By (A.5), for any $x + 0.5 \in [0, N]$,

$$x - \frac{N-1}{2} = (x + 0.5) - \frac{N}{2} = \sum_{u=1}^{\infty} a_u \cos\left(\frac{u\pi(x + 0.5)}{N}\right).$$

Then the numerator of (A.4) is

$$\begin{aligned} &\sum_{i=1}^{N} \left(W(x_{i1} \oplus b) - \frac{N-1}{2}\right)\left(W(x_{ij} \oplus b) - \frac{N-1}{2}\right) \\ &\quad = \sum_{u=1}^{\infty} \sum_{v=1}^{\infty} a_u a_v s(u, v) = \frac{16N^2}{\pi^4} \sum_{\text{odd } u} \sum_{\text{odd } v} \frac{1}{u^2 v^2} s(u, v), \end{aligned} \tag{A.6}$$

where

$$s(u, v) = \sum_{i=1}^{N} \cos\left(\frac{u\pi(W(x_{i1} \oplus b) + 0.5)}{N}\right) \cos\left(\frac{v\pi(W(x_{ij} \oplus b) + 0.5)}{N}\right).$$

By (2.1), for any $x = 0, \dots, N-1$, $\cos(u\pi(W(x)+0.5)/N) = \cos(u\pi(2x+0.5)/N)$. Then

$$s(u,v) = \sum_{i=1}^{N} \cos\left(\frac{u\pi(2x_{i1}+2b+0.5)}{N}\right)\cos\left(\frac{v\pi(2x_{ij}+2b+0.5)}{N}\right)$$

$$(A.7)\qquad = \frac{1}{2}\sum_{i=1}^{N}\cos\left(\frac{2\pi((jv+u)i+c_1)}{N}\right) + \frac{1}{2}\sum_{i=1}^{N}\cos\left(\frac{2\pi((jv-u)i+c_2)}{N}\right),$$

where $c_1 = (b+0.25)(u+v)$ and $c_2 = (b+0.25)(v-u)$. For positive odd numbers u and v, let $I_1 = \{(u,v) : u = jv \text{ or } -jv, v \neq 0 \pmod N\}$ and $I_2 = \{(u,v) : u = 0 \text{ and } v = 0 \pmod N\}$. For $(u,v) \in I_1$, $|s(u,v)| \le N/2$ because only one of the two items in (A.7) can be nonzero. For $(u,v) \in I_2$, $|s(u,v)| \le N$; for $(u,v) \notin I_1 \cup I_2$, $s(u,v) = 0$. Then by (A.3), (A.4) and (A.6),

$$\rho_{\text{ave}}(E_b) = \frac{\sum_{j=2}^{N-1} |\sum_{i=1}^{N}(W(x_{i1}\oplus b) - \frac{N-1}{2})(W(x_{ij}\oplus b)-\frac{N-1}{2})|}{(N-2)(N^3-N)/12}$$

$$(A.8)\qquad \le \frac{192N^2}{\pi^4(N^3-N)(N-2)}\sum_{j=2}^{N-1}\left(\sum_{I_1}\frac{N}{2}\frac{1}{u^2v^2} + \sum_{I_2} N\frac{1}{u^2v^2}\right)$$

$$= \frac{192N^2}{\pi^4(N^2-1)(N-2)}\sum_{j=2}^{N-1}\left(\sum_{I_1}\frac{1}{2u^2v^2} + \sum_{I_2}\frac{1}{u^2v^2}\right).$$

Since

$$\sum_{j=2}^{N-1}\left(\sum_{I_1}\frac{1}{2u^2v^2} + \sum_{I_2}\frac{1}{u^2v^2}\right)$$
$$\le \frac{1}{2}\sum_{\text{odd } v}\frac{1}{v^2}\left(2\sum_{\text{odd } u}\frac{1}{u^2} - \sum_{k=0}^{\infty}\frac{1}{(v+2kN)^2} - 2\sum_{\text{odd } k}\frac{1}{k^2N^2}\right)$$
$$\le \sum_{\text{odd } v}\frac{1}{v^2}\sum_{\text{odd } u}\frac{1}{u^2} - \frac{1}{2}\sum_{\text{odd } v}\frac{1}{v^4} - \frac{1}{N^2}\sum_{\text{odd } v}\frac{1}{v^2}\sum_{\text{odd } k}\frac{1}{k^2}$$
$$= \frac{N^2-1}{N^2}\left(\frac{\pi^4}{8^2}\right) - \frac{\pi^4}{192},$$

where we used the fact that $\sum_{\text{odd } v} 1/v^2 = \pi^2/8$ and $\sum_{\text{odd } v} 1/v^4 = \pi^4/96$. Then by (A.8),

$$\rho_{\text{ave}}(E_b) \le \frac{1}{N-2}\frac{192N^2}{\pi^4(N^2-1)}\left(\frac{N^2-1}{N^2}\left(\frac{\pi^4}{8^2}\right) - \frac{\pi^4}{192}\right)$$
$$= \frac{1}{N-2}\left(3 - \frac{N^2}{N^2-1}\right) < \frac{2}{N-2}. \qquad \square$$

PROOF OF THEOREM 6. For any $b = 0, \dots, N-1$, let $E_b = (e_{ij})$. Because $\sum_{i=1}^{N}(e_{ij} - (N-1)/2)^2 = N(N^2-1)/12$ for any $j = 1, \dots, N-1$, by Theorem 5, we have

$$\sum_{j=2}^{N-1}\left|\sum_{i=1}^{N}\left(e_{i1} - \frac{N-1}{2}\right)\left(e_{ij} - \frac{N-1}{2}\right)\right| < \frac{N(N^2-1)}{6}. \tag{A.9}$$

Let ρ_{jk}^* be the correlation between the jth and kth columns of E_b^*. Similar to (A.3),

$$\rho_{\text{ave}}(E_b^*) = \frac{\sum_{j=2}^{N-1}|\rho_{1j}^*|}{N-2}. \tag{A.10}$$

Note that

$$\rho_{1j}^* = \frac{12C_0}{N(N-1)(N-2)} \tag{A.11}$$

with

$$\begin{aligned} C_0 = &\sum_{\substack{e_{i1}<W(b)\\ e_{ij}<W(b)}}(e_{i1}-\mu)(e_{ij}-\mu) + \sum_{\substack{e_{i1}>W(b)\\ e_{ij}<W(b)}}(e_{i1}-1-\mu)(e_{ij}-\mu) \\ &+ \sum_{\substack{e_{i1}<W(b)\\ e_{ij}>W(b)}}(e_{i1}-\mu)(e_{ij}-1-\mu) \\ &+ \sum_{\substack{e_{i1}>W(b)\\ e_{ij}>W(b)}}(e_{i1}-1-\mu)(e_{ij}-1-\mu) \\ = &\sum_{i=1}^{N}\left(e_{i1} - \frac{N-1}{2}\right)\left(e_{ij} - \frac{N-1}{2}\right) + C_1 + C_2, \end{aligned}$$

where $\mu = (N-2)/2$,

$$\begin{aligned} C_1 = &\frac{1}{2}\left(\sum_{e_{i1}<W(b)} e_{ij} - \sum_{e_{i1}>W(b)} e_{ij} + \sum_{e_{ij}<W(b)} e_{i1} - \sum_{e_{ij}>W(b)} e_{i1}\right) \\ &+ \frac{(N-1)^2}{4} - (W(b))^2 \end{aligned}$$

and

$$C_2 = \frac{1}{4}\Bigg(\sum_{\substack{e_{i1}<W(b)\\ e_{ij}<W(b)}} 1 + \sum_{\substack{e_{i1}>W(b)\\ e_{ij}>W(b)}} 1 - \sum_{\substack{e_{i1}>W(b)\\ e_{ij}<W(b)}} 1 - \sum_{\substack{e_{i1}<W(b)\\ e_{ij}>W(b)}} 1\Bigg).$$

It is easy to see that $|C_1| \le (N^2-1)/4$ and $|C_2| \le (N-1)/4$. Hence, by (A.9), (A.10) and (A.11),

$$\begin{aligned}\rho_{\text{ave}}(E_b^*) &< \frac{12}{N(N-1)(N-2)^2} \\ &\quad \times \left(\frac{N(N^2-1)}{6} + \frac{(N-2)(N^2-1)}{4} + \frac{(N-2)(N-1)}{4}\right) \\ &< \frac{5(N+1)}{(N-2)^2}.\end{aligned}$$

□

PROOF OF THEOREM 7. The proof is similar to that of Theorem 5. By (A.5), for $j = 1, \dots, (N-1)/2$,

$$\sum_{i=1}^{N}\left(w(x_{i1}) - \frac{N}{2}\right)\left(w(x_{ij}) - \frac{N}{2}\right) = \frac{16N^2}{\pi^4}\sum_{\text{odd } v}\frac{1}{u^2v^2}s(u,v),$$

where

$$s(u,v) = \sum_{i=1}^{N}\cos\left(\frac{u\pi w(x_{i1})}{N}\right)\cos\left(\frac{v\pi w(x_{ij})}{N}\right).$$

Similar to (A.8), we can prove that

$$\sum_{j=2}^{(N-1)/2}\left|\sum_{i=1}^{N}\left(w(x_{i1}) - \frac{N}{2}\right)\left(w(x_{ij}) - \frac{N}{2}\right)\right| \le \frac{N^3}{24}.$$

Since

$$\begin{aligned}&\sum_{i=1}^{N-1}\left(w(x_{i1}) - \frac{N+1}{2}\right)\left(w(x_{ij}) - \frac{N+1}{2}\right) \\ &\quad = \sum_{i=1}^{N}\left(w(x_{i1}) - \frac{N}{2}\right)\left(w(x_{ij}) - \frac{N}{2}\right) \\ &\qquad - (N-1) + \frac{(N+1)^2+1}{4},\end{aligned}$$

then

$$\begin{aligned}
&\sum_{j=2}^{(N-1)/2}\left|\sum_{i=1}^{N-1}\left(w(x_{i1})-\frac{N+1}{2}\right)\left(w(x_{ij})-\frac{N+1}{2}\right)\right| \\
&\quad\le \frac{N^3}{24}+\left(\frac{N-1}{2}-1\right)\left(\frac{(N+1)^2+1}{4}-(N-1)\right) \\
&\quad= \frac{N^3}{6}-\frac{5N^2-12N+18}{8} \\
&\quad\le \frac{(N+1)(N-1)(N-3)}{6}.
\end{aligned}$$

Hence,

$$\begin{aligned}
\rho_{\text{ave}}(H) &= \rho_{\text{ave}}\bigl(w(A_1)\bigr) \\
&= \frac{\sum_{j=2}^{(N-1)/2}|\sum_{i=1}^{N-1}(w(x_{i1})-\frac{N+1}{2})(w(x_{ij})-\frac{N+1}{2})|}{(m-1)(N+1)(N-1)(N-3)/12} \\
&\le \frac{2}{m-1}. \qquad \square
\end{aligned}$$

PROOF OF THEOREM 8. To save space, we sketch only the main steps.

Step 1. For $N=2p$, $\phi(N)=p-1$ and $D=(x_{ij})$ with $x_{ij}=i(2j-1) \pmod N$ for $i=1,\dots,2p$ and $j=1,\dots,p-1$. With proper row and column permutations, D is equivalent to

$$\begin{pmatrix} 2C \\ 2C+p \end{pmatrix} \pmod N, \tag{A.12}$$

where $C=(y_{ij})$ is an $p\times(p-1)$ GLP design with $y_{ij}=i\cdot j \pmod p$ for $i=1,\dots,p$ and $j=1,\dots,p-1$. Then $E_b=W(D_b)$ is equivalent to

$$\tilde{E}_b=\begin{pmatrix} W(2C\oplus b) \\ W\bigl(2C\oplus(b+p)\bigr) \end{pmatrix}.$$

Step 2. Consider $W(2C\oplus b)$. If b is even, $2C\oplus b=2(C+b/2 \pmod p)$. Then $w(2C\oplus b)=2w_p(C+b/2 \pmod p)$ where w is the modified Williams transformation defined in (2.2) and w_p is the modified transformation with N replaced by p. By Lemma 2 and Theorem 1, $d_{ik}(w(2C\oplus b))=2[d_{ik}(w_p(C+b/2 \pmod p)))]=2(N^2-1)/3$ for $i\ne k$, $i\ne p$, $k\ne p$, and $i+k\ne p$. Following the lines of Lemma 2 will result $d_{ik}(W(2C\oplus b))=d_{ik}(w(2C\oplus b))$. Then

$$d_{ik}\bigl(W(2C\oplus b)\bigr)=\bigl(N^2-4\bigr)/6 \qquad \text{for } i\ne k, i\ne p, k\ne p, \text{ and } i+k\ne p. \tag{A.13}$$

If b is odd, $W(2C\oplus b)=N-1-W(2C\oplus(b+p))$ and (A.13) also holds.

Step 3. If b is even, the last row of $W(2C \oplus b)$ is $(2b, \dots, 2b)$ and each other row is a permutation of $\{0, 3, 4, \dots, 2(p-1)-1, 2(p-1)\}\backslash\{2b\}$. Based on this structure, we get

$$d_{ip}\big(W(2C \oplus b)\big) = \frac{N^2}{6} - \frac{N+2}{4} + \frac{W(b)}{2} + \frac{g(b)}{2}, \tag{A.14}$$

$$d_{i(p-i)}\big(W(2C \oplus b)\big) = \frac{N^2}{6} + \frac{N}{2} - 1 - W(b) - g(b), \tag{A.15}$$

where

$$g(b) = \left(W(b) - \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right)N\right)\left(W(b) - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)N\right).$$

Similarly, if b is odd, (A.14) and (A.15) also hold.

Step 4. Because $W(2C \oplus b) = N - 1 - W(2C \oplus (b+p))$, $W(2C \oplus (b+p))$ has the same distance structure as $W(2C \oplus b)$.

Step 5. By the structure of $W(2C \oplus (b+p))$ and $W(2C \oplus b)$, by computation, we can get

$$d_{i(p+k)}\big(\tilde{E}(b)\big) = \begin{cases} N^2/4 - l_1(b) & \text{for } i = k \neq p; \\ (N/2-1)l_1(b) & \text{for } i = k = p; \\ N^2/6 - l_1(b) + 1/3 & \text{for } (i,k) \in I_1; \\ N^2/6 - (N-2)/4 + l_2(b)/2 - l_1(b) & \text{for } (i,k) \in I_2; \\ -N^2/12 + (N/2-1)l_1(b) + N/2 - l_2(b) & \text{for } (i,k) \in I_3, \end{cases} \tag{A.16}$$

where $l_1(b) = |N - 2W(b) - 1|$, $l_2(b) = W(b) + g(b)$, $I_1 = \{(i,k) : i \neq p, k \neq p, i+k \neq p\}$, $I_2 = \{(i,k) : i \neq p, k = p, \text{ or } i = p, k \neq p\}$ and $I_3 = \{(i,k) : i \neq p, k \neq p, i+k = p\}$.

Step 6. For $b = \lfloor N(1+1/\sqrt{3})/4 \rfloor$, $W(b) = 2b = \lfloor N(1+1/\sqrt{3})/2 \rfloor$ or $\lfloor N(1+1/\sqrt{3})/2 \rfloor + 1$, so $-N/\sqrt{3} \leq g(b) \leq 0$. Then $l_1(b) = O(N)$ and $l_2(b) = O(N)$. Since for any $N \times (N/2-1)$ LHD, $d_{\text{upper}} = (N+1)(N-2)/6$, by (A.13)–(A.16), it can be verified that $d_{\text{eff}}(E_b) = d_{\text{eff}}(\tilde{E}_b) = 1 - O(1/N)$. □

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