



A new non-iterative deterministic algorithm for constructing asymptotically orthogonal maximin distance Latin hypercube designs

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Abstract

Latin hypercube designs (LHDs), maximin distance designs (MDDs) and orthogonal designs (ODs) are becoming popular and preferred choices in many areas of scientific investigation. A LHD has good projective properties on any single dimension for its uniform coverage of each individual factor, but it does not guarantee good space-filling properties in higher dimensions. A MDD maximizes the distances between its points and thus achieves the space-filling property in the full-dimensional space, but it does not guarantee the orthogonality of its factors. ODs are useful because they ensure the estimates of linear effects are uncorrelated. Since each of these three designs has pros and cons from different perspectives, a design that combines their benefits will be far superior to each design on its own. This paper gives a new non-iterative deterministic algorithm for constructing asymptotically orthogonal maximin distance LHDs. Compared with the existing results, the newly constructed LHDs have a much better performance in any dimension. Theoretical and numerical justifications for the optimality behavior of the newly constructed LHDs are given. Moreover, an iterative algorithm utilizing a mixture of criteria is provided for further improvement of the performance of the newly constructed LHDs from multiple perspectives.

Keywords Latin hypercube designs · Orthogonal designs · Maximin distance designs

Mathematics Subject Classification 62K05 · 62K15

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1 Introduction

Latin hypercube designs (LHDs) (McKay et al., 1979) are becoming popular and preferred choices for designing experiments, especially computer experiments, due to their uniform coverage of each individual factor (Fang et al., 2006; Santner et al., 2003). A LHD is an $n \times s$ matrix, denoted as $LHD(n, s)$, whose columns are permutations of $\left\{-\frac{n-1}{2}, -\frac{n-3}{2}, \dots, \frac{n-3}{2}, \frac{n-1}{2}\right\}$. From the perspective of experimental design, the columns are called factors, the rows are called runs and the values are called levels. If each level appears exactly $\frac{n}{q}$ times, it is called a U -type design with n runs, s factors and q levels, denoted as $U(n, q^s)$. Developing new efficient techniques for constructing optimal U -type designs from various optimality perspectives is one of the hot topics recently (cf. Elsawah and Fang, 2020; Elsawah, 2022a). A $LHD(n, s)$ is a U -type design with $q = n$. Since a LHD scatters the representative points of each individual factor in an intelligent manner to cover the experimental region well, it has good projective properties on any single dimension. However, there is no guarantee that a full-dimensional LHD (i.e., all the s factors together) has good space-filling properties when it is randomly generated. From the perspective of statistics, we can simply conclude that LHDs guarantee uniform samples for the marginal distribution of each single input, however there is no guarantee that they will have good multivariate properties.

A maximin distance design (MDD) (Johnson et al., 1990) maximizes the distances between the experimental points by maximizing the minimum L_2 -distance (ML_2D) so that no two points are too close. For any $LHD(n, s)$ with n rows $r_i = (r_{i1}, \dots, r_{is})$, $1 \leq i \leq n$, its ML_2D is defined as follows

$$ML_2D(LHD(n, s)) = \min \left\{ L_2D_{ij} = \sum_{k=1}^s |r_{ik} - r_{jk}|^2 : |r_i \neq r_j, |r_i, r_j \in LHD(n, s) \right\}.$$

A MDD maximizes the ML_2D value among all the ML_2D values over the experimental domain. Therefore, a MDD achieves the space-filling property in the full-dimensional space that cannot be guaranteed by a randomly generated LHD. Moreover, a MDD is asymptotically D-optimal under the Gaussian process model (Johnson et al., 1990). The construction of maximin distance LHDs (MDLHDs) has received a significant attention in the past few years and many techniques have been presented, interested reader can refer to Tang (1994); Van Dam et al. (2007); Zhou and Xu (2015); Joseph et al. (2015); Lin and Kang (2016); Wang et al. (2018). It is worth-mentioning that the level-permutation technique can be employed to enhance the space-filling behavior of a constructed design (cf. Elsawah, 2022b). For first-order polynomial models, orthogonal LHDs (OLHDs) are useful because they ensure the estimates of linear effects are uncorrelated. However, a space-filling LHD in terms of distance (i.e., MDLHD) may not be an OLHD and vice versa (Joseph & Hung, 2008). This fact is investigated in Sect. 5.

Orthogonality is a significant criterion for evaluating designs that estimate more effects without confounding. A design is called orthogonal if the correlation coefficient between any two distinct columns in the design is zero. For any $LHD(n, s)$ with s columns $c_j = (c_{1j}, \dots, c_{nj})$, $1 \leq j \leq s$, its orthogonality can be measured as follows

$$\rho_{max}(LHD(n, s)) = \max \{ \rho_{ij}(LHD(n, s)) = \rho(c_i, c_j) : c_i \neq c_j, c_i, c_j \in LHD(n, s) \},$$

where

$$\rho(c_i, c_j) = \left| \frac{\sum_{k=1}^n (c_{ki} - \bar{c}_i)(c_{kj} - \bar{c}_j)}{\sqrt{\sum_{k=1}^n (c_{ki} - \bar{c}_i)^2 \sum_{k=1}^n (c_{kj} - \bar{c}_j)^2}} \right| \text{ and } \bar{c}_i = \sum_{k=1}^n \frac{c_{ki}}{n}.$$

A design is called an orthogonal design (OD), if $\rho_{max} = 0$. If $\rho_{max} \neq 0$ but very close to zero, it is called a nearly OD. The construction of OLHDs and ODs has received a significant attention in the past few years and many techniques have been given, interested reader can refer to Ye (1998); Steinberg and Lin (2006); Cioppa and Lucas (2007); Bingham et al. (2009); Pang et al. (2009); Georgiou (2009); Lin et al. (2009, 2010); Sun et al. (2009, 2010, 2011); Yang and Liu (2012); Georgiou and Efthimiou (2014); Elsawah et al. (2021); Wang et al. (2022); Weng et al. (2023); Ke et al. (2023).

Recently, Pang et al. (2022) presented a new non-iterative technique for constructing asymptotically MDLHDs with $2^{\alpha+1}$ runs and $3 \times 2^{\alpha-1}$ factors, $LHD(2^{\alpha+1}, 3 \times 2^{\alpha-1})$, $\alpha \geq 2$. This paper improves the technique in Pang et al. (2022) and gives a new non-iterative deterministic algorithm for constructing nearly orthogonal MDLHDs (OMDLHDs) with $2^{\alpha+1}$ runs and $3 \times 2^{\alpha-1}$ factors. The newly constructed LHDs are better than the existing LHDs that can be generated via the non-iterative algorithm in Pang et al. (2022) and the iterative algorithm using the SA2008 function in the R package LHD (cf. Joseph and Hung, 2008). The newly constructed LHDs are OMDLHDs for large numbers of runs and factors. The numerical results show that for $\alpha \geq 10$, the newly constructed LHDs are optimal in view of orthogonality and ML_2D , i.e., they are OMDLHDs. Theoretical and numerical justifications for the optimality behavior of the newly constructed LHDs are given. For further improvement of the performance of the newly constructed LHDs, an iterative algorithm is given based on a mixture of orthogonality and ML_2D criteria.

The rest of this paper is organized as follows. Section 2 gives the new non-iterative deterministic construction algorithm for asymptotically OMDLHDs. Sections 3 and 4 investigate the behavior of the newly constructed LHDs in view of the orthogonality and L_2 -distance, respectively. An iterative algorithm for improving the performance of the newly constructed LHDs is discussed in Sect. 5. We close through the conclusion and future work in Sect. 6. For clarity and due to the limitation of the space, we relegate the all figures (cf. Figs. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17) and all the proofs to an Appendix.

2 A non-iterative algorithm for asymptotically OMDLHDs

Sun et al. (2009) presented a new construction technique for OLHDs with $2^{\alpha+1}$ runs and 2^α factors $LHD(2^{\alpha+1}, 2^\alpha)$, $\alpha \geq 2$ with a fold-over structure. Readers who are interested in reading more about fold-over techniques for symmetric and asymmetric designs can refer to Elsayah and Qin (2017) and Elsayah (2017), respectively and the references therein. Recently, Wang et al. (2015) gave two techniques (cf. Algorithm 1 and Algorithm 2 in Wang et al., 2015) to add more columns to any LHD with a fold-over structure. The power of the combination of the techniques in Sun et al. (2009) and Wang et al. (2015) is investigated in this paper to construct asymptotically OMDLHDs with $2^{\alpha+1}$ runs and $3 \times 2^{\alpha-1}$ factors $LHD(2^{\alpha+1}, 3 \times 2^{\alpha-1})$, $\alpha \geq 2$, called \mathcal{L}_α^{new} , by constructing OLHDs via the technique in Sun et al. (2009) and then following Algorithm 2 in Wang et al. (2015) to add more columns as follows.

Algorithm 1: Constructing asymptotically OMDLHDs

- **Step 1:** For an integer $\alpha \geq 2$, generate the following two $2^\alpha \times 2^\alpha$ matrices

$$\mathcal{A}_\alpha = \begin{pmatrix} \mathcal{A}_{\alpha-1} & -\mathcal{A}_{\alpha-1}^* \\ \mathcal{A}_{\alpha-1} & \mathcal{A}_{\alpha-1}^* \end{pmatrix} \text{ and } \mathcal{B}_\alpha = \begin{pmatrix} \mathcal{B}_{\alpha-1} & -\mathcal{B}_{\alpha-1}^* - 2^{\alpha-1} \mathcal{A}_{\alpha-1}^* \\ \mathcal{B}_{\alpha-1} + 2^{\alpha-1} \mathcal{A}_{\alpha-1} & \mathcal{B}_{\alpha-1}^* \end{pmatrix},$$

where $\mathcal{A}_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, $\mathcal{B}_1 = \begin{pmatrix} 1 & 2 \\ 2 & -1 \end{pmatrix}$ and $\mathcal{M}^* = \begin{pmatrix} -\mathcal{M}_1 \\ \mathcal{M}_2 \end{pmatrix}$ for any $n \times m$

matrix $\mathcal{M} = \begin{pmatrix} \mathcal{M}_1 \\ \mathcal{M}_2 \end{pmatrix}$ with even n and \mathcal{M}_1 and \mathcal{M}_2 are the top and bottom half, respectively.

- **Step 2:** Generate a $2^{\alpha+1} \times 2^\alpha$ matrix with a fold-over structure by combining the matrices \mathcal{A}_α and \mathcal{B}_α as follows

$$\mathcal{C}_\alpha = \begin{pmatrix} \mathcal{B}_\alpha - \frac{1}{2} \mathcal{A}_\alpha \\ \frac{1}{2} \mathcal{A}_\alpha - \mathcal{B}_\alpha \end{pmatrix}.$$

- **Step 3:** Generate the following $2^{\alpha+1} \times 2^{\alpha-1}$ matrix

$$\mathcal{H}_\alpha^{new} = \begin{pmatrix} \mathcal{E}_{\alpha-1} \\ \mathcal{F}_{\alpha-1} \end{pmatrix},$$

where $\mathcal{E}_{\alpha-1} = (\mathcal{E}_{ij})$, $\mathcal{F}_{\alpha-1} = (\mathcal{F}_{ij})$, $\mathcal{C}_{\alpha-1} = (\mathcal{C}_{ij})$, $\mathcal{S}_{\mathcal{C}_{\alpha-1}} = (\mathcal{S}_{ij})$,

$$\mathcal{S}_{ij} = \begin{cases} +1, & \text{if } \mathcal{C}_{ij} \geq 0; \\ -1, & \text{if } \mathcal{C}_{ij} < 0 \end{cases} \text{ and}$$

$$\begin{cases} \mathcal{E}_{ij} = \mathcal{S}_{ij}(2|\mathcal{C}_{ij}| - \frac{1}{2}), \mathcal{F}_{ij} = \mathcal{S}_{ij}(2|\mathcal{C}_{ij}| + \frac{1}{2}), & \text{for } 1 \leq i \leq 2^{\alpha-1}; \\ \mathcal{E}_{ij} = \mathcal{S}_{ij}(2|\mathcal{C}_{ij}| + \frac{1}{2}), \mathcal{F}_{ij} = \mathcal{S}_{ij}(2|\mathcal{C}_{ij}| - \frac{1}{2}), & \text{for } 2^{\alpha-1} + 1 \leq i \leq 2^\alpha. \end{cases}$$

- **Step 4:** The newly constructed $LHD(2^{\alpha+1}, 3 \times 2^{\alpha-1})$ is given by column-combining the two matrices \mathcal{C}_α and \mathcal{H}_α^{new} as follows $\mathcal{L}_\alpha^{new} = (\mathcal{C}_\alpha \ \mathcal{H}_\alpha^{new})$.

Remark 1 Pang et al. (2022) constructed $LHD(2^{\alpha+1}, 3 \times 2^{\alpha-1})$, $\alpha \geq 2$, called $\mathfrak{L}_\alpha^{P22}$, by constructing OLHDs via the technique in Sun et al. (2009) and then following Algorithm 1 in Wang et al. (2015) as follows

$$\mathfrak{L}_\alpha^{P22} = (C_\alpha \mathcal{H}_\alpha^{P22}), \mathcal{H}_\alpha^{P22} = \begin{pmatrix} 2C_{\alpha-1} - \frac{1}{2}\mathbf{1}_{C_{\alpha-1}} \\ 2C_{\alpha-1} + \frac{1}{2}\mathbf{1}_{C_{\alpha-1}} \end{pmatrix},$$

where C_α is generated as mentioned-above and $\mathbf{1}_{C_{\alpha-1}}$ is an all-ones matrix with the same size as $C_{\alpha-1}$.

An illustrative example. To understand the mechanism of the above-mentioned algorithms, Table 1 gives the $A_\alpha, B_\alpha, C_\alpha, \mathcal{H}_\alpha^{P22}, \mathfrak{L}_\alpha^{P22}, \mathcal{H}_\alpha^{new}$ and $\mathfrak{L}_\alpha^{new}$ for $\alpha = 2$. From Table 1, we get: (i) $ML_2D(\mathfrak{L}_2^{new}) = 55 > ML_2D(\mathfrak{L}_2^{P22}) = 52$, $ML_2D(\mathcal{H}_2^{new}) = ML_2D(\mathcal{H}_2^{P22}) = 2$ and $2^{nd}ML_2D(\mathcal{H}_2^{new}) = 13 > 2^{nd}ML_2D(\mathcal{H}_2^{P22}) = 10$, where $2^{nd}ML_2D$ is the second minimum L_2 -distance. (ii) $\rho_{max}(\mathfrak{L}_2^{new}) = \rho_{max}(\mathfrak{L}_2^{P22}) = 0.1904$, $\rho_{max}(\mathcal{H}_2^{new}) = 0 < \rho_{max}(\mathcal{H}_2^{P22}) = 0.047$ and $\rho_{mean}(\mathfrak{L}_2^{new}) = 0.037 < \rho_{mean}(\mathfrak{L}_2^{P22}) = 0.039$, where ρ_{mean} is the mean of all the absolute correlation values among the factors. That is, the newly constructed LHD \mathfrak{L}_2^{new} is better than the existing LHD \mathfrak{L}_2^{P22} in terms of the L_2 -distances among their runs and the correlations among their factors. The forthcoming discussions provide more numerical and theoretical investigations to support this interesting finding.

Lemma 1 For any j -th column $L_j = (L_{1,j}, \dots, L_{2^{\alpha+1},j})^T$, $\alpha \geq 2$, $1 \leq j \leq 3 \times 2^{\alpha-1}$ of the newly constructed LHD $\mathfrak{L}_\alpha^{new}$, we get the following interesting behavior: (a) L_j is a permutation of $\left\{ -\frac{2^{\alpha+1}-1}{2}, -\frac{2^{\alpha+1}-3}{2}, \dots, \frac{2^{\alpha+1}-3}{2}, \frac{2^{\alpha+1}-1}{2} \right\}$ for any $\alpha \geq 2$ and $1 \leq j \leq 3 \times 2^{\alpha-1}$. (b) $|L_{i,j} + L_{2^{\alpha}+i,j}| = 0$ for any $1 \leq i \leq 2^\alpha$ and $1 \leq j \leq 2^\alpha$. (c) $|L_{i,j} - L_{2^{\alpha}+i,j}| = 1$ for any $1 \leq i \leq 2^\alpha$ and $2^\alpha + 1 \leq j \leq 3 \times 2^{\alpha-1}$. (d) $|L_{i,j} - L_{k,j}| \geq 1$ for any $1 \leq i, k \leq 2^\alpha$ and $1 \leq j \leq 3 \times 2^{\alpha-1}$.

3 Investigating the orthogonality of the newly constructed LHDs

This section investigates the correlations among the factors of the newly constructed LHDs. A comparison study between the existing LHDs by Pang et al. (2022) (cf. Remark 1) and the newly constructed LHDs via the new proposed Algorithm 1 is given. All the theoretical proofs are given in the Appendix.

Lemma 2 From the above-mentioned Algorithm 1, it is obvious that: (i) The designs C_α and \mathcal{H}_α^{new} are LHDs with a fold-over structure, i.e., they can be written as follows

$(d^T - d^T)^T$. **(ii)** The design C_α is an orthogonal LHD, i.e., the correlation between any i -th column and j -th column is $\rho_{\max}(C_\alpha) = \rho_{ij}(C_\alpha) = 0, 1 \leq i \neq j \leq 2^\alpha$.

Theorem 1 The newly constructed LHDs $\mathcal{H}_\alpha^{\text{new}}$ are orthogonal LHDs, however the existing LHDs \mathcal{H}_α^{P22} are nearly orthogonal LHDs, where for any $\alpha \geq 2$ we get

$$\rho_{\max}(\mathcal{H}_\alpha^{\text{new}}) = \rho_{ij}(\mathcal{H}_\alpha^{\text{new}}) = 0 < \rho_{\max}(\mathcal{H}_\alpha^{P22}) = \rho_{ij}(\mathcal{H}_\alpha^{P22}) = \frac{3}{4^{\alpha+1} - 1}, 1 \leq i \neq j \leq 2^{\alpha-1}.$$

Theorem 2 The newly constructed LHDs $\mathcal{L}_\alpha^{\text{new}} = (C_\alpha \mathcal{H}_\alpha^{\text{new}})$ are asymptotically OLHDs, where

$$\rho_{\max}(\mathcal{L}_\alpha^{\text{new}}) \rightarrow 0 \text{ as } \alpha \rightarrow \infty.$$

To provide numerical justifications for the above-mentioned theoretical main findings, Table 2 gives the maximum ρ_{\max} and mean ρ_{mean} of the correlations correlations $|\rho_{ij}|, 1 \leq i \neq j \leq 3 \times 2^{\alpha-1}$ between each two factors of the $3 \times 2^{\alpha-1}$ factors of the existing LHDs \mathcal{L}_α^{P22} and the newly constructed LHDs $\mathcal{L}_\alpha^{\text{new}}$ for $2 \leq \alpha \leq 10$. For a closer look and greater understanding, all the $\binom{3 \times 2^{\alpha-1}}{2}$ correlations $|\rho_{ij}|, 1 \leq i \neq j \leq 3 \times 2^{\alpha-1}$ for \mathcal{L}_α^{P22} and $\mathcal{L}_\alpha^{\text{new}}$ are given in Figs. 1, 2, 3, 4 for $2 \leq \alpha \leq 5$. From Table 2 and Figs. 1, 2, 3, 4, we can conclude that: **(i)** The correlations among the $3 \times 2^{\alpha-1}$ factors of the newly constructed LHDs $\mathcal{L}_\alpha^{\text{new}}$ are less than those among the factors of the existing LHDs \mathcal{L}_α^{P22} , where $\rho_{\text{mean}}(\mathcal{L}_\alpha^{\text{new}}) < \rho_{\text{mean}}(\mathcal{L}_\alpha^{P22})$ (cf. the in-depth justification in Remark A1 in the Appendix). **(ii)** The existing LHDs \mathcal{L}_α^{P22} and the newly constructed LHDs $\mathcal{L}_\alpha^{\text{new}}$ are nearly orthogonal LHDs with the same maximum correlation values, where $\rho_{\max}(\mathcal{L}_\alpha^{P22}) = \rho_{\max}(\mathcal{L}_\alpha^{\text{new}})$. **(iii)** The efficiency in terms of the orthogonality increases as α increases, where

Table 2 The orthogonality of the newly constructed LHDs $\mathcal{L}_\alpha^{\text{new}}$ compared with the existing LHDs \mathcal{L}_α^{P22} for $2 \leq \alpha \leq 10$

α	size	$\rho_{\max} = \max\{\rho_{ij}, i \neq j\}$		$\rho_{\text{mean}} = \text{mean}\{\rho_{ij}, i \neq j\}$	
		\mathcal{L}_α^{P22}	$\mathcal{L}_\alpha^{\text{new}}$	\mathcal{L}_α^{P22}	$\mathcal{L}_\alpha^{\text{new}}$
2	8×6	0.1904	0.1904	0.039683	0.037037
3	16×12	0.0941	0.0941	0.010784	0.009804
4	32×24	0.04692	0.04692	0.002810	0.002525
5	64×48	0.02344	0.02344	0.000717	0.000641
6	128×96	0.01171	0.01171	0.000181	0.000161
7	256×192	0.00585	0.00585	0.000046	0.000041
8	512×384	0.00292	0.00292	0.000011	0.000010
9	1024×768	0.00147	0.00147	2.8573×10^{-6}	2.5406×10^{-6}
10	2048×1536	0.00073	0.00073	7.1479×10^{-7}	6.3547×10^{-7}

$\rho_{\max}(\mathfrak{L}_\alpha^{\text{new}}) < \rho_{\max}(\mathfrak{L}_\beta^{\text{new}})$ for any $\alpha > \beta$. Moreover, it is worth-mentioning that $\rho_{\max}(\mathfrak{L}_\alpha^{\text{new}}) \simeq 0$ for any $\alpha \geq 10$.

4 Investigating the L_2 -distance of the newly constructed LHDs

This section investigates the L_2 -distances among the runs of the newly constructed LHDs. A comparison study between the existing LHDs in Pang et al. (2022) (cf. Remark 1) and the newly constructed LHDs via the new proposed Algorithm 1 is given. All the theoretical proofs are given in the Appendix.

Theorem 3 *The design C_α is a MDLHD among all the LHDs with $2^{\alpha+1}$ runs, 2^α factors and a fold-over structure, where*

$$ML_2D(C_\alpha) = \frac{2^{\alpha-1}}{3}(4^{\alpha+1} - 1).$$

Remark 2 From Lemma 2 and Theorem 3, we conclude that the design C_α is an OMDLHD among all the LHDs with $2^{\alpha+1}$ runs, 2^α factors and a fold-over structure.

Lemma 3 *It is worth-mentioning that the LHD C_α has only the following two different L_2 -distance values*

$$L_2D_{ij}(C_\alpha) = \begin{cases} \frac{2^\alpha(4^{\alpha+1}-1)}{3}, & \text{for any } j = i + 2^\alpha \text{ and } 1 \leq i \leq 2^\alpha; \\ \frac{2^{\alpha-1}(4^{\alpha+1}-1)}{3}, & \text{otherwise.} \end{cases}$$

Theorem 4 *The newly constructed LHD $\mathcal{H}_\alpha^{\text{new}}$ and the existing LHD \mathcal{H}_α^{P22} have the same ML_2D , which is the L_2 -distance between the i -th run and the $j(=i + 2^\alpha)$ -th run, where*

$$ML_2D(\mathcal{H}_\alpha^{\text{new}}) = ML_2D(\mathcal{H}_\alpha^{P22}) = 2^{\alpha-1}.$$

Theorem 5 *The ML_2D of the newly constructed LHD $\mathfrak{L}_\alpha^{\text{new}}$ is larger than the ML_2D of the existing LHD $\mathfrak{L}_\alpha^{P22}$, where*

$$ML_2D(\mathfrak{L}_\alpha^{\text{new}}) = 2^{3\alpha} - 2^{2\alpha-1} - 2^{\alpha-2} > ML_2D(\mathfrak{L}_\alpha^{P22}) = 2^{3\alpha} - \frac{3}{4}2^{2\alpha}.$$

Moreover, the difference between them is given as follows

$$ML_2D(\mathfrak{L}_\alpha^{\text{new}}) - ML_2D(\mathfrak{L}_\alpha^{P22}) = 4^{\alpha-1} - 2^{\alpha-2} > 0.$$

Table 3 The ML_2D of the newly constructed LHDs \mathcal{L}_α^{new} compared with the existing LHDs \mathcal{L}_α^{P22} for $2 \leq \alpha \leq 10$

α	size	\mathcal{L}_α^{P22}	\mathcal{L}_α^{new}	$\mathcal{L}_\alpha^{new} - \mathcal{L}_\alpha^{P22}$	$UB = \lfloor 2^{3\alpha} + 2^{2\alpha-1} \rfloor$	$eff(\mathcal{L}_\alpha^{new})$
2	8×6	52	55	3	72	0.764
3	16×12	464	478	14	544	0.88
4	32×24	3904	3964	60	4224	0.94
5	64×48	32000	32248	248	33280	0.97
6	128×96	259072	260080	1008	264192	0.98
7	256×192	2084864	2088928	4064	2105344	0.992
8	512×384	16728064	16744384	16320	16809984	0.996
9	1024×768	134021120	134086528	65408	134348800	0.998
10	2048×1536	1072955392	1073217280	261888	1074266112	0.999 ≈1

Theorem 6 *The newly constructed LHDs \mathcal{L}_α^{new} are asymptotically MDLHDs, where the efficiency is given as follows*

$$eff(\mathcal{L}_\alpha^{new}) \rightarrow 1 \text{ as } \alpha \rightarrow \infty.$$

To provide numerical justifications for the above-mentioned theoretical main findings, Table 3 gives the ML_2D between any two runs of all the $2^{\alpha+1}$ runs of the existing LHDs \mathcal{L}_α^{P22} and the newly constructed LHDs \mathcal{L}_α^{new} for $2 \leq \alpha \leq 10$. Moreover, the upper bound of the ML_2D , $UB = \lfloor 2^{3\alpha} + 2^{2\alpha-1} \rfloor$, where $\lfloor \zeta \rfloor$ is the integral part of ζ (cf. Zhou and Xu (2015)), and the corresponding efficiency of the newly constructed LHDs are calculated in Table 3. For a closer look and greater understanding, all the $\binom{2^{\alpha+1}}{2} L_2$ -distances L_2D_{ij} between each two runs of all the $2^{\alpha+1}$ runs of the LHDs \mathcal{C}_α for $2 \leq \alpha \leq 4$ are given in Fig. 5; all the $\binom{2^{\alpha+1}}{2} L_2$ -distances between each two runs of all the $2^{\alpha+1}$ runs of the existing LHDs \mathcal{H}_α^{P22} and the newly constructed LHDs \mathcal{H}_α^{new} for $2 \leq \alpha \leq 4$ are given in Figs. 6, 7, 8; and all the $\binom{2^{\alpha+1}}{2} L_2$ -distances between each two runs of all the $2^{\alpha+1}$ runs of \mathcal{L}_α^{P22} and \mathcal{L}_α^{new} for $2 \leq \alpha \leq 4$ are given in Figs. 9, 10, 11. From Table 3 and Figs. 5, 6, 7, 8, 9, 10, 11, we can conclude that: (i) For any $\alpha \geq 2$, the LHD \mathcal{C}_α has only two different L_2 -distance values. (ii) For any $\alpha \geq 2$, the newly constructed LHD \mathcal{H}_α^{new} and the existing LHD \mathcal{H}_α^{P22} have the same ML_2D , however the $2^{nd} ML_2D$ of the newly constructed LHD \mathcal{H}_α^{new} is larger than the $2^{nd} ML_2D$ of the existing LHD \mathcal{H}_α^{P22} . (iii) The newly constructed LHDs \mathcal{L}_α^{new} is better than the existing LHDs \mathcal{L}_α^{P22} , where $ML_2D(\mathcal{L}_\alpha^{new}) > ML_2D(\mathcal{L}_\alpha^{P22})$. (iv) The efficiency in terms of the ML_2D increases as α increases, where $eff(\mathcal{L}_\alpha^{new}) > eff(\mathcal{L}_\beta^{new})$ for any $\alpha > \beta$. Moreover, it is worth-mentioning that $eff(\mathcal{L}_\alpha^{new}) \simeq 1$ for any $\alpha \geq 10$.

5 An iterative algorithm for improving the new LHDs

As we can see from the foregoing discussions, the maximum pairwise correlation between the factors and the minimum L_2 -distance between the points are both good criteria for generating efficient LHDs. It is thought that minimizing correlation should spread out the points and maximizing the distance between the points should reduce the correlation. However, the practice demonstrated that each criterion has its advantages and disadvantages from different perspectives and there is no one-to-one relationship between them and designs obtained by them can be quite different (cf. Joseph and Hung (2008)). Figure 12 illustrates this fact for randomly generated 100 LHDs with 10 factors and 8 runs. Thus, it is still hard to classify LHDs based on these two criteria and there is a need to present a new criterion or investigate a new perspective at the use of these two efficient criteria. A bi-objective criterion ($CorML_2D$) for constructing nearly OMDLHDs can be defined for the newly constructed LHD \mathbf{L} with $2^{\alpha+1}$ runs and $3 \times 2^{\alpha-1}$ factors as follows

$$CorML_2D_{\omega}(\mathbf{L}) = \omega(1 - \rho_{max}(\mathbf{L})) + (1 - \omega) \frac{ML_2D(\mathbf{L})}{[2^{3\alpha} + 2^{2\alpha-1}]}, \quad 0 \leq \omega \leq 1.$$

The optimal LHD $\mathbf{L}^{optimal}$ from the set of all the possible LHDs \mathcal{U} with the same size maximizes $CorML_2D_{\omega}$ for a given ω over all the LHDs in \mathcal{U} , i.e.,

$$CorML_2D_{\omega}(\mathbf{L}^{optimal}) = \max_{\mathbf{L} \in \mathcal{U}} (CorML_2D_{\omega}(\mathbf{L})).$$

Therefore, it obvious that: (i) The optimal LHD $\mathbf{L}^{optimal}$ is an OLHD if $\omega = 1$ and a MDLHD if $\omega = 0$. (ii) When ω is close to 0, the new bi-objective criterion $CorML_2D_{\omega}$ is more sensitive to the ML_2D criterion, where they are directly proportional (cf. Fig. 13). (iii) When ω is close to 1, the new bi-objective criterion $CorML_2D_{\omega}$ is more sensitive to the orthogonality criterion, where they are inversely proportional (cf. Fig. 14). (iv) The new bi-objective criterion $CorML_2D_{\omega}$ is more sensitive to the ML_2D criterion than the orthogonality criterion (cf. Fig. 15).

To provide numerical justifications of the powerful of the new criterion, Fig. 16 and Table 4 give the new bi-objective criterion $CorML_2D_{\omega}$ for the existing LHDs $\mathbf{L}_{\alpha}^{P22}$ and the newly constructed LHDs $\mathbf{L}_{\alpha}^{new}$ for $2 \leq \alpha \leq 10$ and $0 \leq \omega \leq 1$. From Table 4 and Fig. 16, we get that the newly constructed LHDs $\mathbf{L}_{\alpha}^{new}$ are better than the existing LHDs $\mathbf{L}_{\alpha}^{P22}$ in terms of the orthogonality (i.e., ω close to 1); the ML_2D (i.e., ω close to 0); and a mixture of orthogonality and ML_2D (i.e., ω close to 0.5). It is worth-mentioning that when $\omega = 1$, $CorML_2D_1(\mathbf{L}_{\alpha}^{P22}) = CorML_2D_1(\mathbf{L}_{\alpha}^{new})$, which means that $\mathbf{L}_{\alpha}^{P22}$ and $\mathbf{L}_{\alpha}^{new}$ have the same maximum correlation that is consistent with the result in Sect. 3. Moreover, this new criterion can be combined with an iterative algorithm for further improvement of the performance of the newly constructed LHDs.

The threshold accepting (TA) algorithm (cf. Fang et al., 2000) and adjusted TA algorithm (cf. Fang et al., 2017) are widely used efficient iterative algorithms for generating as optimal as possible design from a randomly generated initial design. When the initial design is good (as optimal as possible), an optimal (better than

Table 4 The new bi-objective criterion of the newly constructed LHDs L_{α}^{new} compared with the existing LHDs L_{α}^{P22} for $2 \leq \alpha \leq 10$

ω	$CorML_2D_{\omega}$			$CorML_2D_{\omega}$			$CorML_2D_{\omega}$		
	α	L_{α}^{P22}	L_{α}^{new}	α	L_{α}^{P22}	L_{α}^{new}	α	L_{α}^{P22}	L_{α}^{new}
0.0		0.7222222	0.7638889		0.8529412	0.8786765		0.9242424	0.9384470
0.1		0.7309524	0.7684524		0.8582353	0.8813971		0.9271261	0.9399102
0.2		0.7396825	0.7730159		0.8635294	0.8841176		0.9300098	0.9413734
0.3		0.7484127	0.7775794		0.8688235	0.8868382		0.9328935	0.9428366
0.4		0.7571429	0.7821429		0.8741176	0.8895588		0.9357771	0.9442999
0.5	2	0.7658730	0.7867063	3	0.8794118	0.8922794	4	0.9386608	0.9457631
0.6		0.7746032	0.7912698		0.8847059	0.8950000		0.9415445	0.9472263
0.7		0.7833333	0.7958333		0.8900000	0.8977206		0.9444282	0.9486895
0.8		0.7920635	0.8003968		0.8952941	0.9004412		0.9473118	0.9501527
0.9		0.8007937	0.8049603		0.9005882	0.9031618		0.9501955	0.9516160
1.0		0.8095238	0.8095238		0.9058824	0.9058824		0.9530792	0.9530792
0.0		0.9615385	0.9689904		0.9806202	0.9844356		0.9902724	0.9922027
0.1		0.9630403	0.9697470		0.9813862	0.9848201		0.9906592	0.9923965
0.2		0.9645421	0.9705037		0.9821522	0.9852046		0.9910460	0.9925903
0.3		0.9660440	0.9712603		0.9829183	0.9855891		0.9914328	0.9927841
0.4		0.9675458	0.9720169		0.9836843	0.9859736		0.9918196	0.9929778
0.5	5	0.9690476	0.9727736	6	0.9844503	0.9863580	7	0.9922065	0.9931716
0.6		0.9705495	0.9735302		0.9852164	0.9867425		0.9925933	0.9933654
0.7		0.9720513	0.9742869		0.9859824	0.9871270		0.9929801	0.9935592
0.8		0.9735531	0.9750435		0.9867485	0.9875115		0.9933669	0.9937530
0.9		0.9750549	0.9758001		0.9875145	0.9878960		0.9937537	0.9939468
1.0		0.9765568	0.9765568		0.9882805	0.9882805		0.9941405	0.9941405
0.0		0.9951267	0.9960976		0.9975610	0.9980478		0.9987799	0.9990237
0.1		0.9953211	0.9961948		0.9976584	0.9980966		0.9988287	0.9990481
0.2		0.9955154	0.9962921		0.9977558	0.9981453		0.9988774	0.9990725
0.3		0.9957098	0.9963894		0.9978532	0.9981940		0.9989262	0.9990968
0.4		0.9959041	0.9964867		0.9979506	0.9982428		0.9989750	0.9991212
0.5	8	0.9960985	0.9965839	9	0.9980481	0.9982915	10	0.9990237	0.9991456
0.6		0.9962929	0.9966812		0.9981455	0.9983402		0.9990725	0.9991700
0.7		0.9964872	0.9967785		0.9982429	0.9983890		0.9991213	0.9991944
0.8		0.9966816	0.9968758		0.9983403	0.9984377		0.9991700	0.9992188
0.9		0.9968759	0.9969730		0.9984377	0.9984864		0.9992188	0.9992432
1.0		0.9970703	0.9970703		0.9985352	0.9985352		0.9992676	0.9992676

the initial one) resulting design can be generated after few iterations. However, when the initial design is not good (far away from optimal), an optimal resulting design cannot be generated after the same number of iterations and more iterations (time) are needed and there is no guarantee that the resulting design will be optimal. Therefore, using as good as possible designs as initial designs is much

better than the randomly generated designs. Since the newly constructed LHDs \mathbb{L}_α^{new} in this paper are nearly optimal from orthogonality and ML_2D , they can be used as initial LHDs for the TA algorithm or adjusted TA algorithm to get much better LHDs from various perspectives. Fig. 17 gives the flowchart of an updated version of the TA algorithm as an iterative algorithm for improving the performance of the newly constructed LHDs in terms of the new bi-objective criterion $CorML_2D_\omega$ for a given ω . It is worth-mentioning that by using the updated version of the TA algorithm in Fig. 17 with small numbers of iterations, we could not get LHDs better than our newly constructed LHDs. Which means that our newly constructed LHDs are optimal LHDs, especially for large sizes.

6 Conclusion and future work

A new construction non-iterative algorithm for nearly orthogonal maximin distance LHDs is given in this paper. The newly constructed LHDs are compared with the existing LHDs in Pang et al. (2022) and appear to perform better than them. The main results show that the newly constructed LHDs are asymptotically orthogonal maximin distance LHDs. Moreover, an iterative algorithm for further improvement of the performance of the newly constructed LHDs is given using a new criterion. Furthermore, the iterative algorithm using the SA2008 function in the R package LHD (cf. Joseph and Hung, 2008) is used to generate LHDs with the same sizes as those for the newly constructed LHDs and ρ_{max} , ρ_{mean} and ML_2D are calculated in Table 5. The results show that, aside from the fact that the SA2008 function generated LHDs too slowly and takes too long time for large sizes, the LHDs that are generated by our new non-iterative algorithm are superior to those that are generated by the SA2008 function in view of orthogonality and L_2 -distance.

There are some other interesting ideas related to this idea for further study, such as: (i) This idea can be extended to generate large nearly orthogonal maximin distance LHDs by combining the technique in this paper with the multiple doubling technique in Elsawah (2021). The initial results show that this idea is a promising idea and the results will be given in the future paper. (ii) The bi-objective criterion can be extended to multi-objective criterion by combining more

Table 5 The orthogonality and ML_2D of the newly constructed LHDs \mathbb{L}_α^{new} compared with the LHDs that are generated using the SA2008 function in the R package LHD

α	size	$\rho_{max} = \max\{\rho_{ij}, i \neq j\}$		$\rho_{mean} = mean\{\rho_{ij}, i \neq j\}$		ML_2D	
		SA2008	\mathbb{L}_α^{new}	SA2008	\mathbb{L}_α^{new}	SA2008	\mathbb{L}_α^{new}
2	8×6	0.3095238	0.1904	0.10582011	0.037037	49	55
3	16×12	0.4088235	0.0941	0.12495915	0.009804	284	478
4	32×24	0.3771994	0.04692	0.09074108	0.002525	2663	3964
5	64×48	0.3191850	0.02344	0.08194182	0.000641	21940	32248
6	128×96	0.2981253	0.01171	0.06657851	0.000161	21940	32248

criteria. For example, Elsayah and Fang (2019) constructed uniform minimum aberration designs by minimizing the generalized word-length pattern (GWLP, cf. Ma and Fang, 2001) and then minimizing the used uniformity criterion. However, combining these two criteria as the above-mentioned bi-objective criterion needs more attention, where the uniformity criterion is a scalar and the GWLP is a sequence. In such cases, the dictionary cross-entropy loss function from Weng et al. (2021) can be used to transfer (simplify) the GWLP from sequence to scalar. The power of the combination of many criteria from this point of view will be investigated in our future work. **(iii)** Suppose that an experimenter begins the experimentation using the newly constructed LHDs. After the experiment is over or during the experimentation, some additional resources become available and the experimenter needs to afford more runs to the design. How does the experimenter pick the additional runs and augment the original LHD so as to get an optimal extended LHD? The future paper will provide an answer to this question by combining the technique in this paper with the augmented techniques in Elsayah et al. (2019)(cf. also Elsayah and Qin, 2016). **(iv)** Finally, the projection properties of the newly constructed LHDs need to be investigated and the relationship between a newly constructed LHD in the full-dimension and its low-dimensional projections will be studied in the light of the results in Elsayah et al. (2019).

Appendix

Proof of Theorem 1 From Theorems 2 and 3 in Wang et al. (2015), we get the following correlations between any i -th column and j -th column of \mathcal{H}_α^{P22} and \mathcal{H}_α^{new}

$$\rho_{ij}(\mathcal{H}_\alpha^{P22}) = \frac{4(2^{2\alpha} - 1)\rho_{ij}(C_{\alpha-1}) + 3}{2^{2\alpha+2} - 1}, \quad 1 \leq i \neq j \leq 2^{\alpha-1} \tag{A1}$$

and

$$\rho_{ij}(\mathcal{H}_\alpha^{new}) = \frac{4(2^{2\alpha} - 1)\rho_{ij}(C_{\alpha-1}) + 3\rho_{ij}(S_{C_{\alpha-1}})}{2^{2\alpha+2} - 1}, \quad 1 \leq i \neq j \leq 2^{\alpha-1}, \tag{A2}$$

respectively. From Lemma 2, we get that $C_{\alpha-1}$ and $S_{C_{\alpha-1}}$ are orthogonal matrices, i.e.,

$$\rho_{ij}(S_{C_{\alpha-1}}) = \rho_{ij}(C_{\alpha-1}) = 0, \quad 1 \leq i \neq j \leq 2^{\alpha-1}. \tag{A3}$$

From (A1)-(A3), the proof can be completed. □

Proof of Theorem 2 From Algorithm 1, we get

$$\rho_{max}(\mathcal{L}_\alpha^{new}) = \max \{ \rho_{max}(C_\alpha), \rho_{max}(C_\alpha, \mathcal{H}_\alpha^{new}), \rho_{max}(\mathcal{H}_\alpha^{new}) \}, \tag{A4}$$

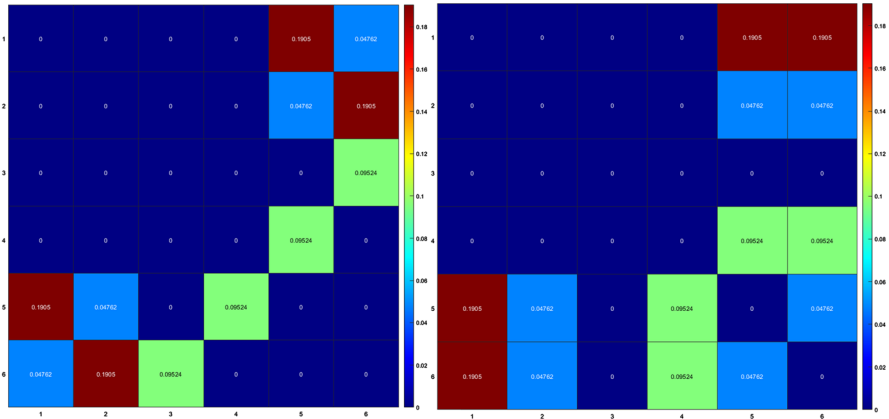


Fig. 1 Correlations among the factors of the newly constructed LHD (\mathcal{L}_α^{new} , left) and the existing LHD (\mathcal{L}_α^{P22} , right) for $\alpha = 2$

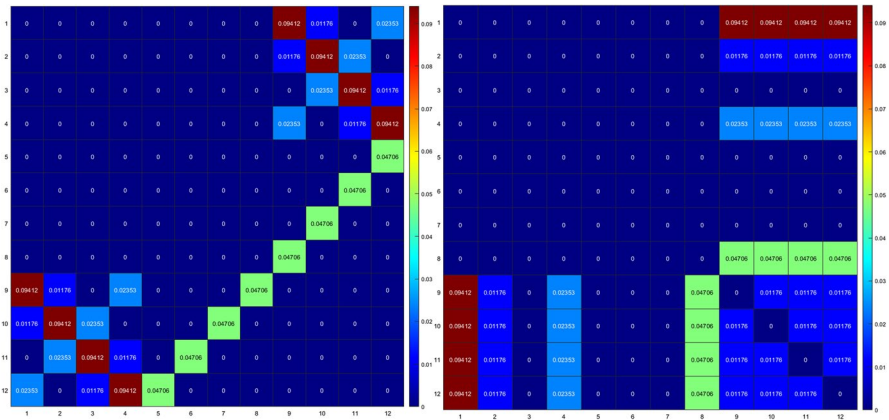


Fig. 2 Correlations among the factors of the newly constructed LHD (\mathcal{L}_α^{new} , left) and the existing LHD (\mathcal{L}_α^{P22} , right) for $\alpha = 3$

where $\rho_{max}(\mathcal{C}_\alpha, \mathcal{H}_\alpha^{new}) = \max\{\rho_{ij}(\mathcal{C}_\alpha, \mathcal{H}_\alpha^{new}), 1 \leq i \leq 2^\alpha, 1 \leq j \leq 2^{\alpha-1}\}$ for any i -th column of \mathcal{C}_α and j -th column of \mathcal{H}_α^{new} . From Theorem 1, Lemma 2 and (A4), we get

$$\rho_{max}(\mathcal{L}_\alpha^{new}) = \rho_{max}(\mathcal{C}_\alpha, \mathcal{H}_\alpha^{new}). \tag{A5}$$

From Theorem 1 in Wang et al. (2015), we get the following upper bound of the correlation between the i -th column of \mathcal{C}_α and any column j satisfying (a) and (c) in Lemma 1 (i.e., column of \mathcal{H}_α^{new})

$$|\rho_{ij}(\mathcal{C}_\alpha, \mathcal{H}_\alpha^{new})| \leq \frac{3 \times 2^\alpha}{2^{2\alpha+2} - 1}. \tag{A6}$$

From (A5) and (A6), we get the following upper bound of the maximum correlation between any distinct columns

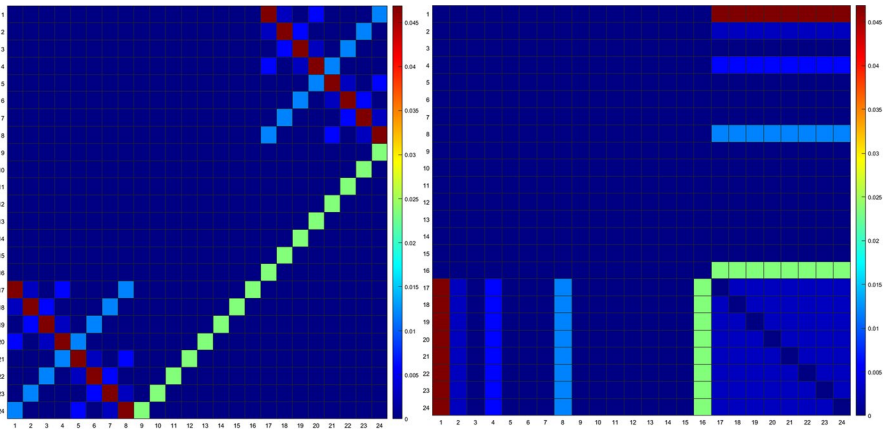


Fig. 3 Correlations among the factors of the newly constructed LHD (\mathcal{L}_α^{new} , left) and the existing LHD (\mathcal{L}_α^{P22} , right) for $\alpha = 4$

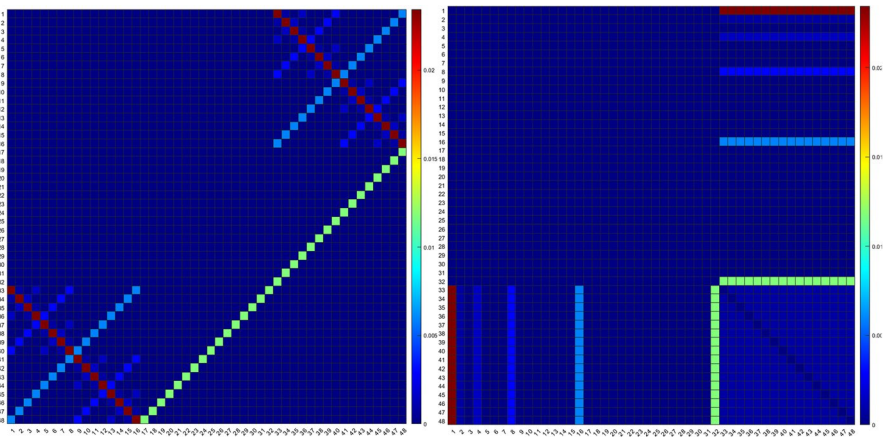


Fig. 4 Correlations among the factors of the newly constructed LHD (\mathcal{L}_α^{new} , left) and the existing LHD (\mathcal{L}_α^{P22} , right) for $\alpha = 5$

$$\rho_{max}(\mathcal{L}_\alpha^{new}) = \max\{\rho_{ij}, 1 \leq i \neq j \leq 2^\alpha + 2^{\alpha-1}\} \leq \frac{3 \times 2^\alpha}{2^{2\alpha+2} - 1}. \tag{A7}$$

From (A7), the proof can be completed. □

Remark A1 From Figs. 1, 2, 3, 4, it is obvious that the set of the correlations among the columns of \mathcal{C}_α and \mathcal{H}_α^{P22}

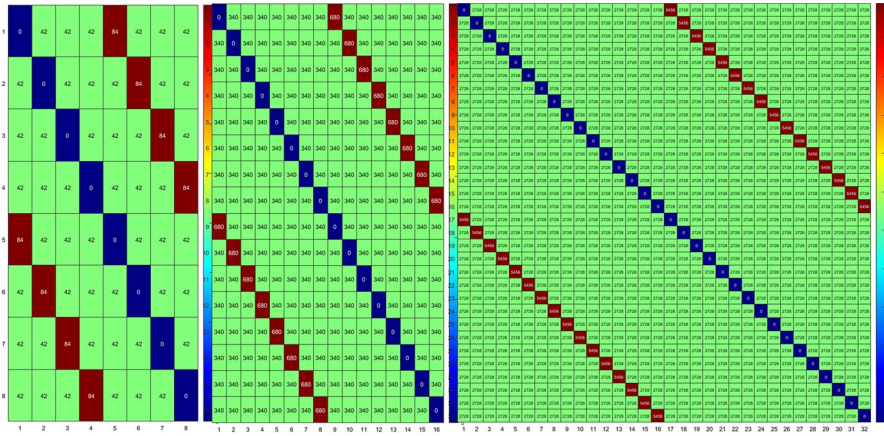


Fig. 5 L_2 -distances among the 2^α runs of the LHD C_α for $\alpha = 2$ (left), $\alpha = 3$ (median) and $\alpha = 3$ (right)

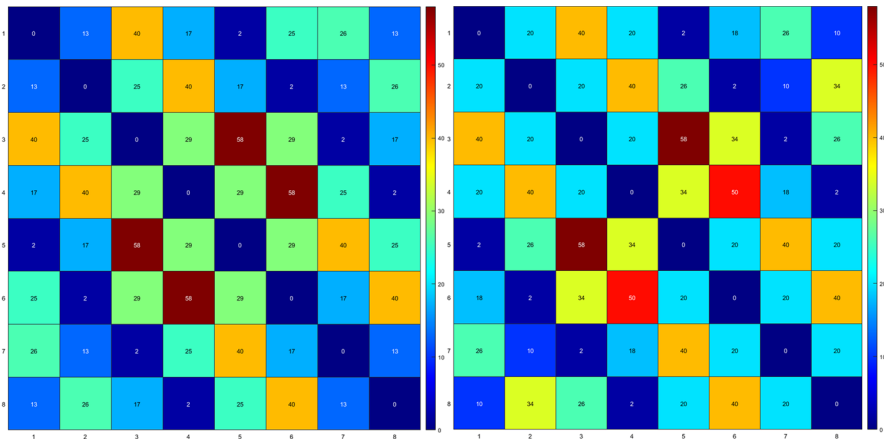


Fig. 6 L_2 -distances among the runs of the newly constructed LHD (\mathcal{H}_α^{new} , left) and the existing LHD (\mathcal{H}_α^{P22} , right) for $\alpha = 2$

$$\{\rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{P22}), 1 \leq i \leq 2^\alpha, 1 \leq j \leq 2^{\alpha-1}\}$$

has the same values as the set of the correlations among the columns of C_α and \mathcal{H}_α^{new}

$$\{\rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{new}), 1 \leq i \leq 2^\alpha, 1 \leq j \leq 2^{\alpha-1}\}.$$

That is,

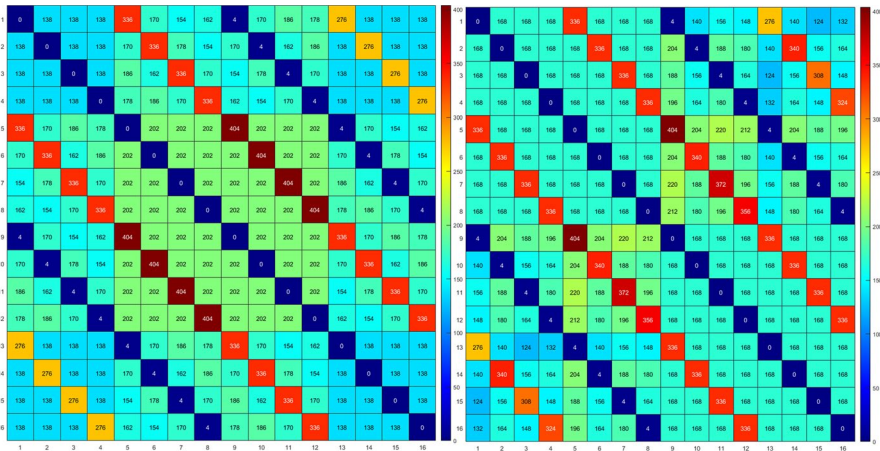


Fig. 7 L_2 -distances among the runs of the newly constructed LHD (\mathcal{H}_α^{new} , left) and the existing LHD (\mathcal{H}_α^{P22} , right) for $\alpha = 3$

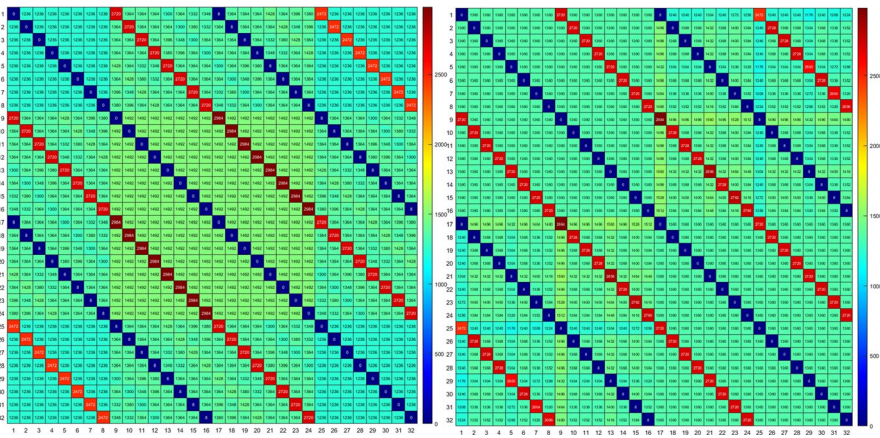


Fig. 8 L_2 -distances among the runs of the newly constructed LHD (\mathcal{H}_α^{new} , left) and the existing LHD (\mathcal{H}_α^{P22} , right) for $\alpha = 4$

$$\sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{P22}) = \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{new}). \tag{A8}$$

From Lemma 2 and Theorem 1, we get

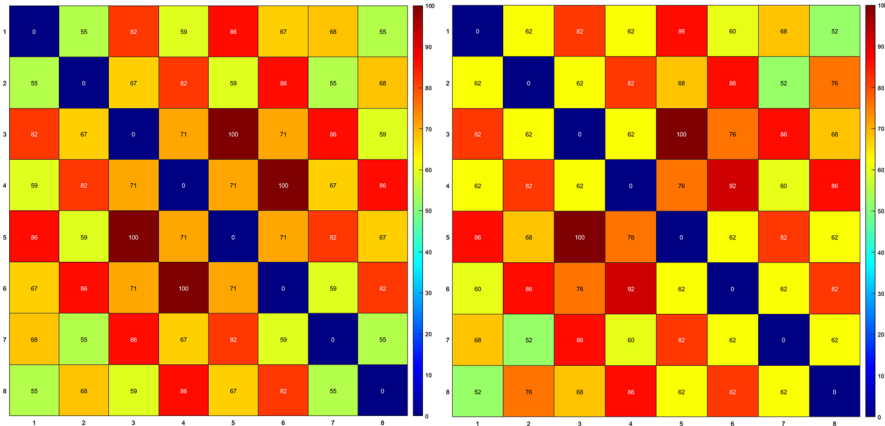


Fig. 9 L_2 -distances among the runs of the newly constructed LHD (\mathbf{L}_α^{new} , left) and the existing LHD (\mathbf{L}_α^{P22} , right) for $\alpha = 2$

$$\begin{aligned}
 \sum_{i(\neq j)=1}^{3 \times 2^{\alpha-1}} \sum_{j=1}^{3 \times 2^{\alpha-1}} \rho_{ij}(\mathbf{L}_\alpha^{new}) &= \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^\alpha} \rho_{ij}(C_\alpha) + \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{new}) \\
 &\quad + \sum_{i(\neq j)=1}^{2^\alpha-1} \sum_{j=1}^{2^\alpha-1} \rho_{ij}(\mathcal{H}_\alpha^{new}) \tag{A9} \\
 &= \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{new}).
 \end{aligned}$$

$$\begin{aligned}
 \sum_{i(\neq j)=1}^{3 \times 2^{\alpha-1}} \sum_{j=1}^{3 \times 2^{\alpha-1}} \rho_{ij}(\mathbf{L}_\alpha^{P22}) &= \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^\alpha} \rho_{ij}(C_\alpha) + \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{P22}) \\
 &\quad + \sum_{i(\neq j)=1}^{2^\alpha-1} \sum_{j=1}^{2^\alpha-1} \rho_{ij}(\mathcal{H}_\alpha^{P22}) \tag{A10} \\
 &= \sum_{i(\neq j)=1}^{2^\alpha} \sum_{j=1}^{2^{\alpha-1}} \rho_{ij}(C_\alpha, \mathcal{H}_\alpha^{P22}) + \sum_{i(\neq j)=1}^{2^\alpha-1} \sum_{j=1}^{2^\alpha-1} \rho_{ij}(\mathcal{H}_\alpha^{P22}).
 \end{aligned}$$

From (A8, A9, A10), we get

$$\rho_{mean}(\mathbf{L}_\alpha^{new}) = mean\{\rho_{ij}(\mathbf{L}_\alpha^{new}), i \neq j\} < \rho_{mean}(\mathbf{L}_\alpha^{P22}) = mean\{\rho_{ij}(\mathbf{L}_\alpha^{P22}), i \neq j\}.$$

Therefore, the newly constructed LHDs \mathbf{L}_α^{new} have correlations among their $3 \times 2^{\alpha-1}$ factors less than the correlations among the $3 \times 2^{\alpha-1}$ factors of the existing LHDs \mathbf{L}_α^{P22} . □

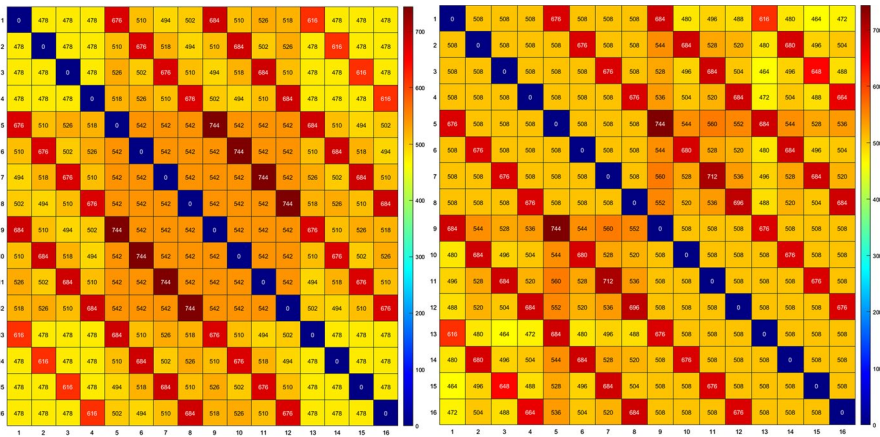


Fig. 10 L_2 -distances among the runs of the newly constructed LHD (L_{α}^{new} , left) and the existing LHD (L_{α}^{P22} , right) for $\alpha = 3$

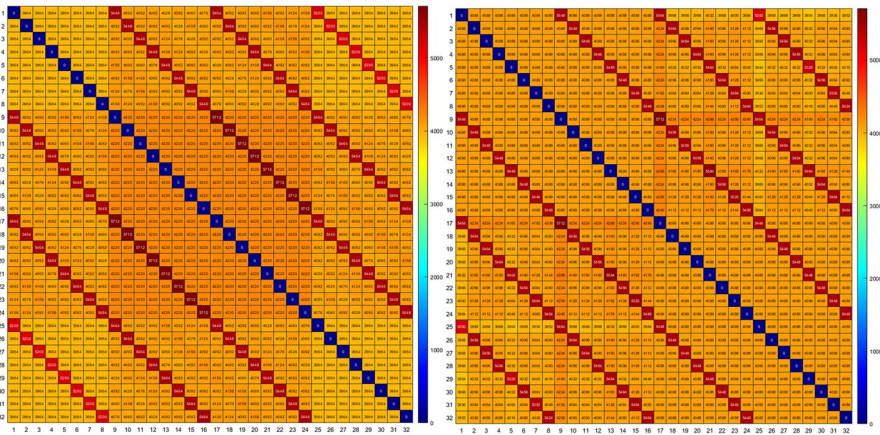


Fig. 11 L_2 -distances among the runs of the newly constructed LHD (L_{α}^{new} , left) and the existing LHD (L_{α}^{P22} , right) for $\alpha = 4$

Proof of Theorem 3 From Lemma 2 in Wang et al. (2018), we get the following upper bound of the ML_2D for any mirror-symmetric U -type design with even number of runs n and s q -level factors $d \in U(n, q^s)$

$$ML_2D(d) \leq \frac{s(q^2 - 1)}{6}. \tag{A11}$$

From Theorem 1 in Wang et al. (2018), a mirror-symmetric U -type design $d \in U(n, q^s)$ with $n = 2s$ achieves this upper bound if it is orthogonal. From Lemma

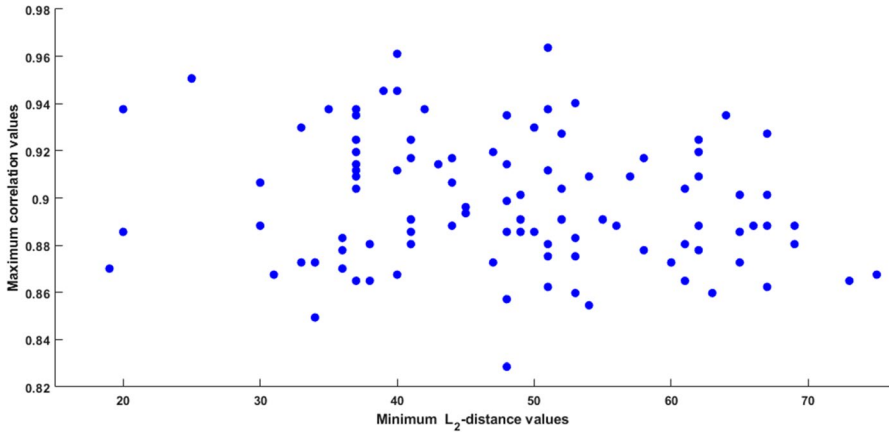


Fig. 12 Maximum correlations vs minimum L_2 -distances for randomly generated 100 LHDs(10,8)

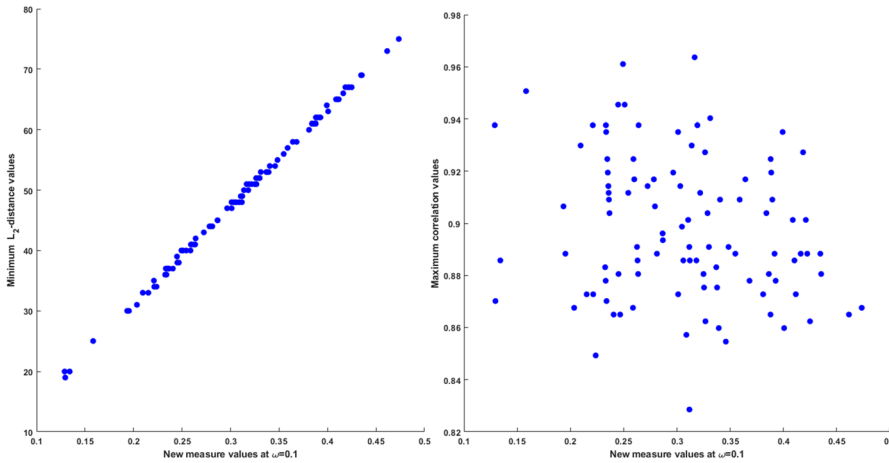


Fig. 13 The new bi-objective criterion vs maximum correlation and minimum L_2 -distance for the randomly generated 100 LHDs(10,8) at $\omega = 0.1$

2, we get \mathcal{C}_α is an orthogonal LHD with fold-over structure (i.e., mirror-symmetric U -type design), $2^{\alpha+1}$ runs and 2^α factors. From (A11) and this discussion, the proof is completed. \square

Proof of Theorem 4 From Lemma 1, for any column $h = (h_1, \dots, h_{2^{\alpha+1}})$ of \mathcal{H}_α^{new} or \mathcal{H}_α^{P22} we get

$$\begin{cases} |h_i - h_j|^2 = 1, & \text{for any } j = i + 2^\alpha \text{ and } 1 \leq i \leq 2^\alpha; \\ |h_i - h_j|^2 \geq 1, & \text{otherwise.} \end{cases} \tag{A12}$$

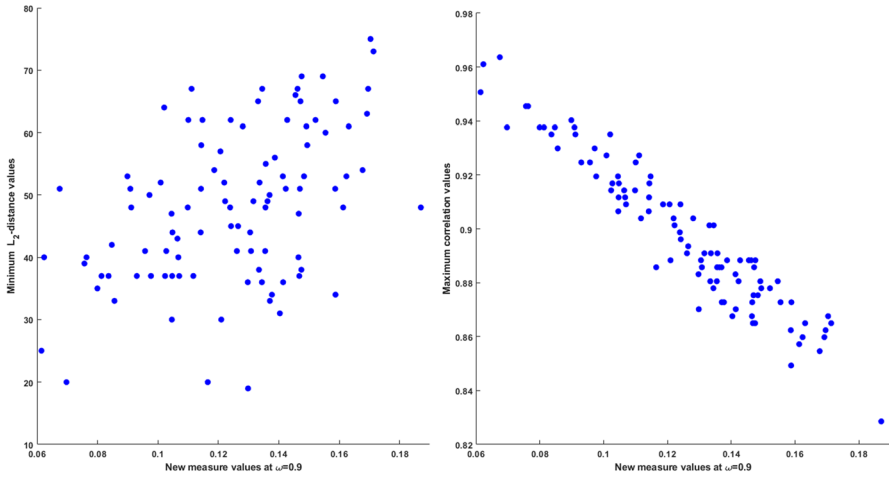


Fig. 14 The new bi-objective criterion vs maximum correlation and minimum L_2 -distance for the randomly generated 100 LHDs(10,8) at $\omega = 0.9$

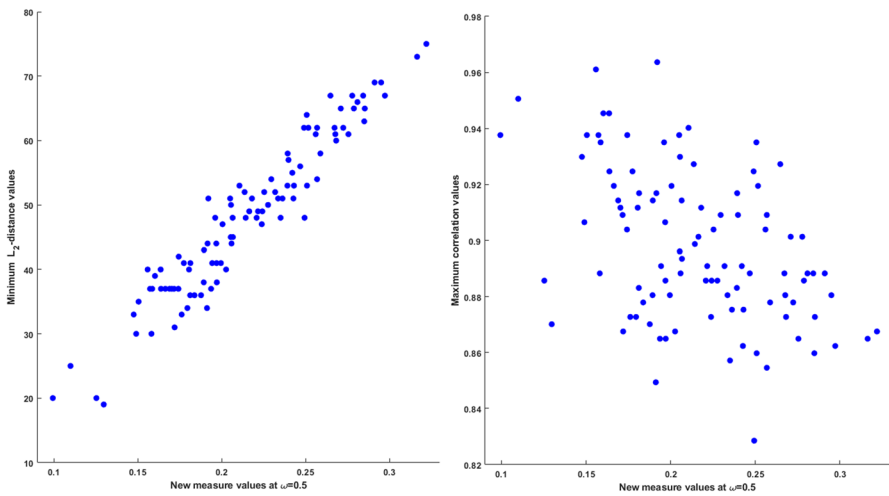


Fig. 15 The new bi-objective criterion vs maximum correlation and minimum L_2 -distance for the randomly generated 100 LHDs(10,8) at $\omega = 0.5$

From (A12), the proof can be completed. □

Proof of Theorem 5 From Theorem 1 in Pang et al. (2022), the $2^{nd} ML_2D$ of the LHD \mathcal{H}_α^{P22} is given as follows

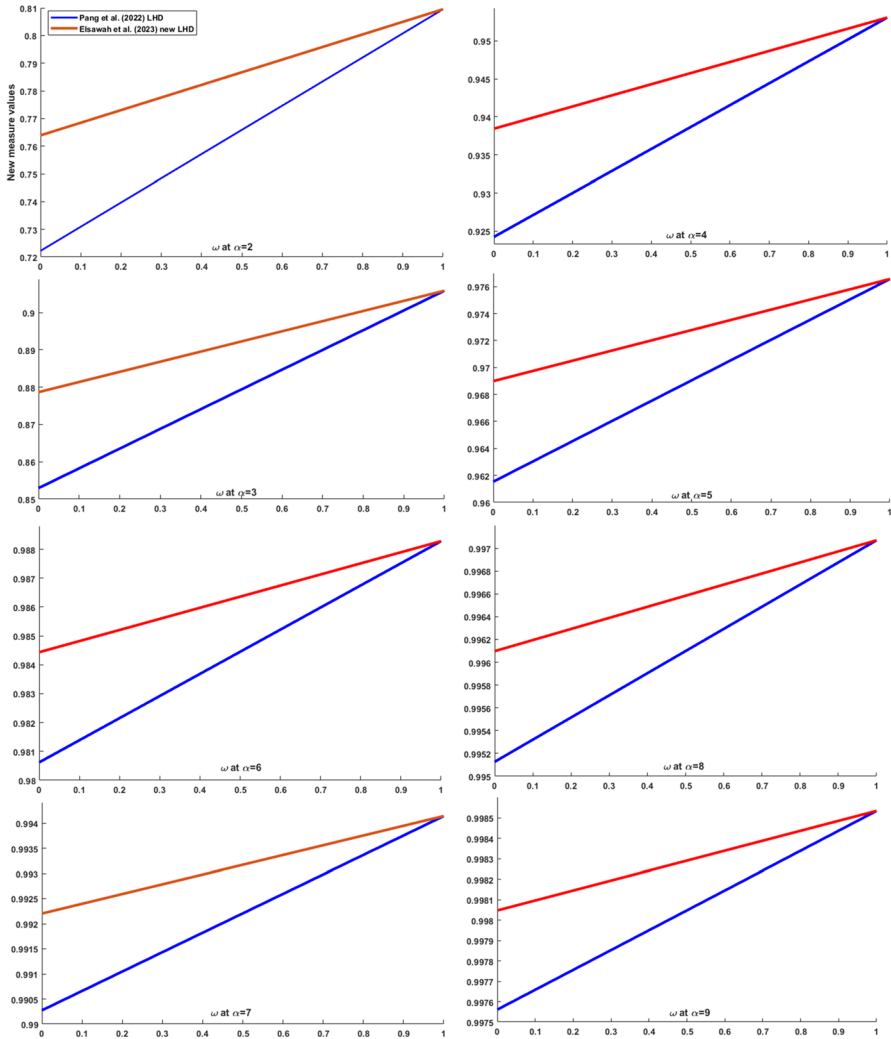


Fig. 16 The new bi-objective criterion of the newly constructed LHDs L_{α}^{new} compared with the existing LHDs L_{α}^{P22} for $2 \leq \alpha \leq 9$

$$2^{nd}ML_2D(\mathcal{H}_{\alpha}^{P22}) = \frac{1}{3}2^{3\alpha} - \frac{3}{4}2^{2\alpha} + \frac{1}{6}2^{\alpha}, \tag{A13}$$

which is achieved only for the runs $i = 1$ and $j = 2^{\alpha} + 2^{\alpha-1} + 2^{\alpha-2} + 1$ and the runs $i = 2^{\alpha-2} + 1$ and $j = 2^{\alpha} + 2^{\alpha-1} + 1$. By the same technique as that in the proof of Theorem 1 in Pang et al. (2022) with some calculations and obvious changes between the new Algorithm 1 in this paper and the algorithm in Pang et al. (2022) (cf. Remark 1), we can get the following $2^{nd}ML_2D$ of the newly constructed LHD $\mathcal{H}_{\alpha}^{new}$

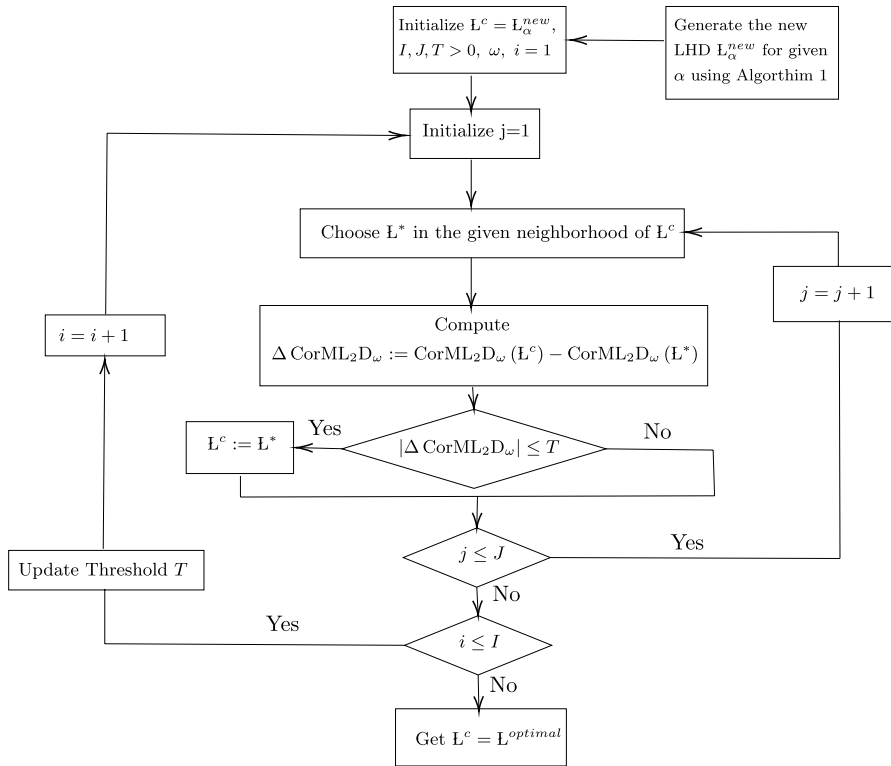


Fig. 17 The flowchart of the iterative algorithm for improving the performance newly constructed LHDs

$$2^{nd}ML_2D(\mathcal{H}_\alpha^{new}) = \frac{1}{3}2^{3\alpha} - 2^{2\alpha-1} - \frac{1}{12}2^\alpha, \tag{A14}$$

which is achieved for the runs $i = 1$ and $j = 2^\alpha + 2^{\alpha-1} + 2^{\alpha-2} + 1$ and the runs $i = 2^{\alpha-2} + 1$ and $j = 2^\alpha + 2^{\alpha-1} + 1$ (cf. Figures 6, 7, 8). From Theorems 3 and 4 and Lemma 3, by the same technique as that in the proof of Theorem 2 in Pang et al. (2022) with some calculations, we get that

$$ML_2D(\mathcal{L}_\alpha^{P22}) = ML_2D(C_\alpha) + 2^{nd}ML_2D(\mathcal{H}_\alpha^{P22}). \tag{A15}$$

$$ML_2D(\mathcal{L}_\alpha^{new}) = ML_2D(C_\alpha) + 2^{nd}ML_2D(\mathcal{H}_\alpha^{new}). \tag{A16}$$

From (A11, A13, A14, A15, A16) with simple calculations, the proof can be completed. □

Proof of Theorem 6 From Zhou and Xu (2015), we get the following upper bound of the ML_2D

$$ML_2D \leq UB = \lfloor 2^{3\alpha} + 2^{2\alpha-1} \rfloor, \lfloor \gamma \rfloor \text{ is the integral part of } \gamma. \quad (\text{A17})$$

From Theorem 5 and (A17), we get

$$\text{eff}(\mathbf{X}_\alpha^{\text{new}}) = \frac{ML_2D(\mathbf{X}_\alpha^{\text{new}})}{UB} = \frac{1}{1 + \left(\frac{1}{2}\right)^{\alpha+1}} - \frac{1}{1 + 2^{\alpha+1}} - \frac{1}{2^{2\alpha+2} + 2^{\alpha+1}}. \quad (\text{A18})$$

From (A18), the proof is completed. \square

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Declarations

Conflict of interest There is no conflict of interest.

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