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CENTERED L_2-DISCREPANCY OF RANDOM SAMPLING AND LATIN HYPERCUBE DESIGN, AND CONSTRUCTION OF UNIFORM DESIGNS

KAI-TAI FANG, CHANG-XING MA, AND PETER WINKER

Abstract. In this paper properties and construction of designs under a centered version of the L_2-discrepancy are analyzed. The theoretic expectation and variance of this discrepancy are derived for random designs and Latin hypercube designs. The expectation and variance of Latin hypercube designs are significantly lower than that of random designs. While in dimension one the unique uniform design is also a set of equidistant points, low-discrepancy designs in higher dimension have to be generated by explicit optimization. Optimization is performed using the threshold accepting heuristic which produces low discrepancy designs compared to theoretic expectation and variance.

1. Introduction

Many problems arising in industry, statistics, physics, and finance require multivariate integration, the canonical form of which can be expressed as

$$I(f) = \int_{C^s} f(\boldsymbol{x}) d\boldsymbol{x}, \tag{1.1}$$

where $C^s = [0,1)^s$ and $f(\boldsymbol{x}) = f(x_1, \cdots, x_s)$. The sample mean method has been recommended to give an approximation to $I(f)$ by

$$\hat{I}(f, \mathcal{P}) = \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{x}_i), \tag{1.2}$$

where $\mathcal{P} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\}$ is a set of points on C^s. If $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n$ are *i.i.d.* uniformly distributed on C^s, the set is called *simple random sampling* or simple random design (SRD) and is denoted by $\mathcal{R}_{n,s}$. It is known that $\hat{I}(f, \mathcal{R}_{n,s})$ is unbiased and has an asymptotic variance $O(n^{-1})$. This rate of convergence is too slow for the applications. Therefore, McKay, Beckman and Conover [MBC79] proposed the so-called *Latin hypercube design* (LHD), which also provides an unbiased estimate $\hat{I}(f, \mathcal{P})$ with smaller asymptotic variance than that of SRD. LHD has been widely used in conducting computer experiments. A systematic study on LHD and various modified versions of LHD that can significantly reduce the asymptotic variance of LHD is given by [Owen92], [Owen94], [Owen95], [KO96], and [Tang93]. In this

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article, we only consider a special case of LHD, where $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n$ are *i.i.d.* uniformly distributed on the lattice set

$$\mathcal{T} = \left\{ \boldsymbol{x} = (x_1, \ldots, x_n) \;\middle|\; \begin{array}{l} x_i = \frac{2a_i - 1}{2n}, i = 1, \ldots, n, \\ (a_1, \ldots, a_n) \text{ is a permutation of } \{1, \ldots, n\} \end{array} \right\}.$$

We denote this LHD by $\mathcal{L}_{n,s}$.

There exist different measures to assess the performance of various designs on C^s. The Koksma-Hlawka inequality gives an upper bound for the approximation error

$$|I(f) - \hat{I}(f, \mathcal{P})| \leq D(\mathcal{P})V(f), \tag{1.3}$$

where $D(\mathcal{P})$ is the discrepancy of $\mathcal{P}$ that will be defined in (1.4), and $V(f)$ is a measure of the variation of f [Nie92]. In fact, we can find a number of other pairs $\{D(\mathcal{P}), V(f)\}$ satisfying the Koksma-Hlawka inequality, where $D(\mathcal{P})$ is a measure of nonuniformity of $\mathcal{P}$ and $V(f)$ is a measure of variation of f. An excellent study on this topic is given by [Hic98]. For SRD, $D(\mathcal{R}_{n,s}) = O(n^{-1/2})$ as $n \to \infty$. The determination of the order of convergence of $D(\mathcal{P})$ for LHD $\mathcal{P}$ is still an open problem. It will be answered for the centered L_2-discrepancy in this paper.

Let $\mathcal{P} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\}$ be a set of n points on $C^s = [0,1)^s$. The star L_p-discrepancy (L_p-discrepancy for simplicity) has been widely used in quasi-Monte Carlo methods (or number-theoretic methods) as well as in uniform design theory (cf. [Nie92] and [FWa94]). It is defined as

$$D_p(\mathcal{P}) = \left\{ \int_{C^s} \left| \frac{N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))}{n} - \mathrm{Vol}([\mathbf{0}, \boldsymbol{x})) \right|^p d\boldsymbol{x} \right\}^{1/p}, \tag{1.4}$$

where $[\mathbf{0}, \boldsymbol{x})$ denotes the interval $[0, x_1) \times \cdots \times [0, x_s)$, $N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))$ the number of points of $\mathcal{P}$ falling in $[\mathbf{0}, \boldsymbol{x})$, and $\mathrm{Vol}(A)$ the volume of A. Among the L_p-discrepancies, the $D_2(\mathcal{P})$ and $D(\mathcal{P}) = D_\infty(\mathcal{P})$ (called discrepancy for short) are used most frequently.

Hickernell [Hic98] pointed out some weakness of the L_p-discrepancy and proposed several modified L_p-discrepancies, among which the centered L_2-discrepancy (CL_2) seems most interesting. Ma and Fang [MF98] and Fang and Mukerjee [FM00] found some connections between CL_2 and orthogonality, minimum aberration, and confounding for a certain class of designs. The centered L_p-discrepancy is a modification of the L_p-discrepancy by the requirement that it becomes invariant under reflections of $\mathcal{P}$ about any plane $x_j = 0.5$. It is defined by

$$(D_p(\mathcal{P}))^p = \sum_{u \neq \emptyset} \int_{C^u} \left| \frac{N(\mathcal{P}_u, J_{\boldsymbol{x}_u})}{n} - \mathrm{Vol}(J_{\boldsymbol{x}_u}) \right|^p du, \tag{1.5}$$

where u is a nonempty subset of the set of coordinate indices $S = \{1, \cdots, s\}$, $|u|$ denotes the cardinality of u, C^u is the $|u|$-dimensional unit cube involving the coordinates in u, $J_{\boldsymbol{x}}$ is an s-dimensional interval uniquely determined by $\boldsymbol{x}$, $\mathcal{P}_u$ is the projection of $\mathcal{P}$ to C^u, and $J_{\boldsymbol{x}_u}$ is the projection of $J_{\boldsymbol{x}}$ on C^u. Let $\mathcal{A}^s$ denote the set of 2^s vertices of the cube C^s and $\alpha = (a_1, \ldots, a_s) \in \mathcal{A}^s$ be the closest one to $\boldsymbol{x}$. Define

$$J_{\boldsymbol{x}} = \{\boldsymbol{y} \in C^s \mid \min(a_j, x_j) \leq y_j < \max(a_j, x_j), \text{ for } 1 \leq j \leq s\}.$$

For CL_2 Hickernell [Hic98] derived an analytical expression

$$
\begin{aligned}
CL_2(\mathcal{P})^2 &= \left(\frac{13}{12}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}(1+\frac{1}{2}|x_{kj}-0.5|-\frac{1}{2}|x_{kj}-0.5|^2) \\
&\quad + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[1+\frac{1}{2}|x_{ki}-0.5|+\frac{1}{2}|x_{ji}-0.5|-\frac{1}{2}|x_{ki}-x_{ji}|\right], \qquad (1.6)
\end{aligned}
$$

where $\boldsymbol{x}_k = (x_{k1}, \cdots, x_{ks}) \in \mathcal{P}$. From the definition (1.5) the centered L_p-discrepancy takes into account not only the uniformity of $\mathcal{P}$ over C^s, but also uniformity of all the projections of $\mathcal{P}$ over C^u.

In Sections 2 and 3 we shall derive the expectation and variance for square CL_2 of simple random designs $\mathcal{R}_{n,s}$ and Latin hypercube designs $\mathcal{L}_{n,s}$, and give comparisons of these statistics. It will be shown that the LHD has much lower expected CL_2-value and variance than SRD. Our results are consistent with the results of comparing variance of $\hat{I}(f,\mathcal{P})$ between SRD and LHD [Owen92]. Note that the LHD $\mathcal{L}_{n,s}$ can be defined in terms of U-type designs.

Definition 1.1. A U-type design U_{n,q^s} is an $n \times s$ matrix $\boldsymbol{U} = (u_{ij})$ of which each column has q entries $1, \ldots, q$ appearing equally often. The induced matrix of $\boldsymbol{U}$, denoted by $\boldsymbol{X_U} = (x_{ij})$, is defined by $x_{ij} = (u_{ij} - 0.5)/q$. When $q = n$, we use the notation $U_{n,s}$ instead of U_{n,n^s}. Let $\mathcal{U}_{n,q^s}$ and $\mathcal{U}_{n,s}$ be the set of all U_{n,q^s} and the set of all $U_{n,s}$, respectively.

Any induced matrix $\boldsymbol{X_U}$ defined in Definition 1.1 corresponds to a set of n points on C^s, denoted by $\mathcal{P}_U$. Each row of $\boldsymbol{X_U}$ corresponds to a point of $\mathcal{P}_U$ on C^s. The $CL_2(\boldsymbol{U})$ is defined as $CL_2(\mathcal{P}_U)$. The LHD $\mathcal{L}_{n,s}$ is a design $\boldsymbol{X_U}$, where $\boldsymbol{U} \in \mathcal{U}_{n,s}$. The design $\boldsymbol{X_U}$, where $\boldsymbol{U} \in \mathcal{U}_{n,q^s}$, can be considered as an extension of LHD and is denoted by $\mathcal{L}_{n,q^s}$. In Sections 2 and 3 we also derive the expectation and variance of $CL_2(\mathcal{L}_{n,q^s})^2$.

The U-type design is the basis of the *uniform design*. The latter is one of "space filling" designs (Cheng and Li (1995) [CL95], and Koehler and Owen (1996) [KO96]). The uniform design allocates experimental points uniformly scattered on the domain in the sense of low-discrepancy [FWa94]. Any discrepancy mentioned before can be used as a measure of nonuniformity. In the past, most uniform designs are obtained in terms of the discrepancy and the L_2-discrepancy. Fang and Winker [FW98] found that both discrepancy and L_2-discrepancy are not suitable measures of nonuniformity for searching the UD, since the discrepancy is not sensitive enough for identifying different designs while the L_2-discrepancy ignores differences $|\frac{N(\mathcal{P},[\boldsymbol{0},\boldsymbol{x}))}{n} - \mathrm{Vol}([\boldsymbol{0},\boldsymbol{x}))|^2$ on any low-dimensional subspace. Therefore, they recommend the use of the three modified L_2-discrepancies proposed by [Hic98]. In this paper we concentrate on the centered L_2-discrepancy for construction of uniform designs.

Let $\mathcal{P}_n$ be the class of sets of n points on C^s. A set $\mathcal{P}^* \in \mathcal{P}_n$ is called a uniform design if it has the smallest CL_2-value over $\mathcal{P}_n$, i.e.,

$$CL_2(\mathcal{P}^*) = \min_{\mathcal{P}\in\mathcal{P}_n} CL_2(\mathcal{P}). \qquad (1.7)$$

In Section 4 we propose a heuristic optimization algorithm for the construction of uniform designs based on U-type designs under CL_2. The results obtained in Sections 2 and 3 provide information which can be used to reduce the computing time of searching uniform designs and low-discrepancy designs.

The paper is organized as follows. The expectation and variance of $CL_2(\mathcal{R}_{n,s})$ and $CL_2(\mathcal{L}_{n,q^s})$ are derived in Sections 2 and 3. Part of the proofs are put into an appendix. Some numerical comparisons of these expectations and variances are also given. In Section 4 we discuss how to construct uniform designs. An algorithm based on threshold accepting is proposed and some modifications are suggested. The performance of this algorithm will be discussed in Section 5, which also provides numerical results for low-discrepancy designs. The last section contains concluding remarks.

2. The expectation of square CL_2 of $\mathcal{R}_{n,s}$ and $\mathcal{L}_{n,s}$

In this section we derive the expectation of square centered L_2-discrepancy for simple random designs $\mathcal{R}_{n,s}$ and Latin hypercube designs $\mathcal{L}_{n,q^s}$. Their difference is also given.

Theorem 2.1. *The average square centered L_2-discrepancy of the random design $\mathcal{R}_{n,s}$ is given by*

$$E(CL_2(\mathcal{R}_{n,s})^2) = \left[\left(\frac{5}{4}\right)^s - \left(\frac{13}{12}\right)^s\right]/n. \tag{2.1}$$

The average square centered L_2-discrepancy of Latin hypercube design $\mathcal{L}_{n,q^s}$ is given by

(2.2)

$$E(CL_2(\mathcal{L}_{n,q^s})^2) = \begin{cases} (\frac{13}{12})^s - 2(\frac{13}{12}-\frac{1}{12q^2})^s + \frac{1}{n}(\frac{5}{4}-\frac{1}{4q^2})^s + (1-\frac{1}{n})(\frac{13}{12}+\frac{n-q^2}{6q^2(n-1)}-\frac{1}{4q^2})^s, & q \text{ odd}, \\ (\frac{13}{12})^s - 2(\frac{13}{12}+\frac{1}{24q^2})^s + \frac{1}{n}(\frac{5}{4})^s + (1-\frac{1}{n})(\frac{13}{12}+\frac{n-q^2}{6q^2(n-1)})^s, & q \text{ even}. \end{cases}$$

Proof. From formula (1.6) and the fact that $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n$ are *i.i.d.* uniformly distributed on C^s, we have

$$\begin{aligned} E(CL_2(\mathcal{R}_{n,s})^2) &= (\frac{13}{12})^s - \frac{2}{n}\sum_{k=1}^n \prod_{j=1}^s E(1+\frac{1}{2}|x_{kj}-0.5| - \frac{1}{2}|x_{kj}-0.5|^2) \\ &\quad + \frac{1}{n^2}\sum_{k=1}^n \prod_{i=1}^s E(1+|x_{ki}-0.5|) \\ &\quad + \frac{2}{n^2}\sum_{k=1}^n \sum_{j=1}^{k-1} \prod_{i=1}^s E\left[1+\frac{1}{2}|x_{ki}-0.5| + \frac{1}{2}|x_{ji}-0.5| - \frac{1}{2}|x_{ki}-x_{ji}|\right] \\ &= (\frac{13}{12})^s - 2\left(1+\int_0^1 (1+\frac{1}{2}|x-0.5| - \frac{1}{2}|x-0.5|^2)dx\right)^s \\ &\quad + \frac{1}{n}\left(\int_0^1 (1+|x-0.5|)dx\right)^s \\ &\quad + \frac{2}{n^2}\frac{n(n-1)}{2}\left(\int_0^1\int_0^1 (1+\frac{1}{2}|x-0.5| + \frac{1}{2}|y-0.5| - \frac{1}{2}|x-y|)dxdy\right)^s \\ &= \left[\left(\frac{5}{4}\right)^s - \left(\frac{13}{12}\right)^s\right]/n. \end{aligned}$$

Thus, equation (2.1) is proved. For giving a proof of formula (2.2) we need the following lemma. Its proof is straightforward and is omitted.

Lemma 2.2.

$$\frac{1}{q}\sum_{i=1}^{q}|\frac{2i-1-q}{2q}| = \begin{cases} \frac{1}{4}-\frac{1}{4q^2}, & q \text{ is odd,} \\ \frac{1}{4}, & q \text{ is even;} \end{cases}$$

$$\frac{1}{q}\sum_{i=1}^{q}(\frac{2i-1-q}{2q})^2 = \frac{1}{12}-\frac{1}{12q^2};$$

$$\frac{1}{q}\sum_{j=1}^{q}\sum_{k=1}^{q}\frac{|j-k|}{q} = \frac{q^2-1}{3q}.$$

Now, we come back to prove formula (2.2).

$$\begin{aligned} E(CL_2(\mathcal{L}_{n,q^s}{}^2) &= (\frac{13}{12})^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}E(1+\frac{1}{2}|x_{kj}-0.5|-\frac{1}{2}|x_{kj}-0.5|^2) \\ &+\frac{1}{n^2}\sum_{k=1}^{n}\prod_{i=1}^{s}E(1+|x_{ki}-0.5|) \\ &+\frac{2}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{k-1}\prod_{i=1}^{s}E\left[1+\frac{1}{2}|x_{ki}-0.5|+\frac{1}{2}|x_{ji}-0.5|-\frac{1}{2}|x_{ki}-x_{ji}|\right] \\ = \quad & (\frac{13}{12})^s - 2\left(\frac{1}{n}\sum_{k=1}^{q}(1+\frac{1}{2}|\frac{2k-1}{2q}-0.5|-\frac{1}{2}|\frac{2k-1}{2q}-0.5|^2)\right)^s \\ &+\frac{1}{n}\left(\frac{1}{q}\sum_{k=1}^{q}(1+|\frac{2k-1}{2q}-0.5|)\right)^s \\ &+\frac{2}{n^2}\frac{n(n-1)}{2}\left(E(1+\frac{1}{2}|x_{ki}-0.5|+\frac{1}{2}|x_{ji}-0.5|-\frac{1}{2}|x_{ki}-x_{ji}|)\right)^s. \end{aligned}$$

Note that

$$\begin{aligned} & E(1+\frac{1}{2}|x_{ki}-0.5|+\frac{1}{2}|x_{ji}-0.5|-\frac{1}{2}|x_{ki}-x_{ji}|) \\ = \quad & \sum_{k=1}^{q}\sum_{j=1}^{q}(1+\frac{1}{2}|\frac{2k-1}{2q}-0.5|+\frac{1}{2}|\frac{2j-1}{2q}-0.5|-\frac{1}{2}|\frac{k-j}{q}|)P(k,j), \end{aligned}$$

where $P(k,j)$ is the probability that the first two elements of a specific column of $\boldsymbol{U}$, where $\boldsymbol{U}$ is uniformly distributed on $\mathcal{U}_{n,q^s}$, are k and j, respectively. Let $r = n/q$ be the duplicate number of each level in each column of $\boldsymbol{U}$. Obviously, we have $P(k,j) = \frac{r^2}{n(n-1)}$ for $k \neq j$, and $P(k,k) = \frac{r(r-1)}{n(n-1)}$. Put these results into the above formula and (2.2) is proved.

From this theorem we immediately have the following corollaries.

Corollary 1. *We have*

$$E(CL_2(\mathcal{L}_{n,q^s})^2) = O(n^{-1}) + O(q^{-2})$$

as $q \to \infty$ *and* $n = q^s \to \infty$.

Corollary 2. *The average square discrepancy of* $\mathcal{L}_{n,s}$ *is*

$$E(CL_2(\mathcal{L}_{n,s})^2) = \begin{cases} (\frac{13}{12})^s - 2(\frac{13}{12} - \frac{1}{12n^2})^s + \frac{1}{n}(\frac{5}{4} - \frac{1}{4n^2})^s + (1-\frac{1}{n})(\frac{13}{12} - \frac{1}{6n} - \frac{1}{4n^2})^s, & n \text{ odd}, \\ (\frac{13}{12})^s - 2(\frac{13}{12} + \frac{1}{24n^2})^s + \frac{1}{n}(\frac{5}{4})^s + (1-\frac{1}{n})(\frac{13}{12} - \frac{1}{6n})^s, & n \text{ even}. \end{cases} \tag{2.3}$$

From (2.1) and (2.3) we can find the difference of average square CL_2-value between simple random designs $\mathcal{R}_{n,s}$ and Latin hypercube designs $\mathcal{L}_{n,s}$.

Corollary 3.

$$\begin{aligned} &E(CL_2(\mathcal{R}_{n,s}))^2 - E(CL_2(\mathcal{L}_{n,s}))^2 \\ &\quad = \left(\frac{13}{12}\right)^{s-1} \frac{s}{6n} - \left(\frac{13}{12}\right)^{s-1} \frac{2s^2+11s}{156n^2} + O(n^{-3}), \end{aligned} \tag{2.4}$$

in particular, when $s = 1$,

$$E(CL_2(\mathcal{R}_{n,1}))^2 - E(CL_2(\mathcal{L}_{n,1}))^2 = \frac{1}{6n} - \frac{1}{12n^2}.$$

This corollary shows that LHDs have a lower expectation of square CL_2-value than that of simple random designs. This result is consistent with the result that the Latin hypercube designs beat random designs in the sense of small-variance [Owen92]. It is not easy to find a sharp upper bound for $CL_2(\mathcal{P}_U)^2$ over $\boldsymbol{U} \in \mathcal{U}_{n,q^s}$. The following example gives a bad U-type design in the sense of uniformity. Therefore, its CL_2 can be considered as an upper bound of $CL_2(\mathcal{P}_U)$, $\boldsymbol{U} \in \mathcal{U}_{n,q^s}$.

Example 2.3. The CL_2 of the U-type design $\mathcal{P}_* = \{(\frac{2i-1}{2n}, \ldots, \frac{2i-1}{2n}), i = 1, \ldots, n\}$ in $[0,1]^s$, where the n points are on a line, is

$$\begin{aligned} (CL_2(\mathcal{P}_*))^2 \quad &= \quad \frac{13}{12} - \frac{2}{n}\sum_{k=1}^{n}(1 + |\frac{2k-1-n}{4n}| - |\frac{2k-1-n}{2n}|^2/2)^s \\ &\quad + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}(1 + |\frac{2k-1}{4n}| + |\frac{2j-1}{4n}| - \frac{|k-j|}{2})^s = O(1). \end{aligned} \tag{2.5}$$

For $s = 2, 3$ and 4, formula (2.5) can be simplified:

$$(CL_2(\mathcal{P}_*))^2 = \begin{cases} \frac{1}{90} + \frac{1}{240}(\frac{50}{n^2} - \frac{11}{n^4}), & s = 2, \\ \frac{2321n^6 + 2390n^4 - 10206n^2 + 360}{60480n^6}, & s = 3, \\ \frac{64427n^8 + 491400n^6 - 322056n^4 + 37080n^2 + 3024}{725760n^8}, & s = 4. \end{cases} \tag{2.6}$$

3. The variance of square CL_2 of $\mathcal{R}_{n,s}$ and $\mathcal{L}_{n,s}$

We have calculated the expectation of $CL_2(\mathcal{R})^2$ and $CL_2(\mathcal{L}_{n,q^s})^2$ in the previous section. In this section, by a similar, but more complicated procedure, we derive the variance of square CL_2 for the random design and Latin hypercube design. As the related proof is too long, we put it into an appendix (found at the end of this article).

Theorem 3.1. *For the random design $\mathcal{R}_{n,s}$ we obtain*

$$\begin{aligned}\mathrm{Var}(CL_2(\mathcal{R}_{n,s})^2) = &\frac{2}{n^2}\left[\left(\frac{19}{16}\right)^s - 2\left(\frac{47}{40}\right)^s + \left(\frac{169}{144}\right)^s\right] \\ &+\frac{1}{n^3}\left[\left(\frac{19}{12}\right)^s - \left(\frac{25}{16}\right)^s - 2\left(\frac{19}{16}\right)^s\right. \\ &\left.+4\left(\frac{65}{48}\right)^s - 4\left(\frac{87}{64}\right)^s + 8\left(\frac{47}{40}\right)^s - 6\left(\frac{169}{144}\right)^s\right].\end{aligned} \tag{3.1}$$

For the Latin hypercube design $\mathcal{L}_{n,q^s}$ we find

$$\begin{aligned}\mathrm{Var}(CL_2(\mathcal{L}_{n,q^s})^2) = &-\left[E(CL_2(\mathcal{L}_{n,q^s}))^2 - \left(\frac{13}{12}\right)^s\right]^2 + \frac{4}{n}(A_1^s + (n-1)A_2^s), \\ &-\frac{4}{n^2}(B_1^s + 2(n-1)B_2^s + (n-1)B_3^s + (n-1)(n-2)B_4^s) \\ &+\frac{1}{n^3}(C_1^s + 4(n-1)C_2^s + (n-1)C_3^s + 2(n-1)C_4^s + 2(n-1)(n-2)C_5^s \\ &+4(n-1)(n-2)C_6^s + (n-1)(n-2)(n-3)C_7^s),\end{aligned} \tag{3.2}$$

where $\delta_q = 1$ for odd q and 0 for even q, and

$$\begin{aligned}A_1 &= \frac{47}{40} + \frac{7+80q^2}{960q^4} - \delta_q\frac{1+16q^2}{64q^4}, \\ A_2 &= \frac{169}{144} - \frac{21+240q^2+4q^4-5n(1+52q^2)}{2880(-1+n)q^4} + \delta_q\frac{3+n+48q^2-52nq^2}{192(-1+n)q^4}, \\ B_1 &= \frac{87}{64} + \frac{1}{32q^2} - \delta_q\frac{1+24q^2}{64q^4}, \\ B_2 &= \frac{47}{40} + \frac{4n-10q^2+70nq^2-59q^4}{320(-1+n)q^4} + \delta_q\frac{3+72q^2-2n(2+37q^2)}{192(-1+n)q^4}, \\ B_3 &= \frac{65}{48} - \frac{6-10n+q^2}{192(-1+n)q^2} + \delta_q\frac{3+72q^2+n(4-82q^2)}{192(-1+n)q^4}, \\ B_4 &= \frac{169}{144} + \frac{5n^2(2+65q^2)+5q^2(18+107q^2)-3n(12+235q^2+88q^4)}{1440(-2+n)(-1+n)q^4} \\ &\quad + \delta_q\frac{-3+2n-72q^2+115nq^2-39n^2q^2}{96(-2+n)(-1+n)q^4}, \\ C_1 &= \frac{19}{12} - \frac{1}{12q^2} - \delta_q\frac{1}{2q^2}, \\ C_2 &= \frac{87}{64} + \frac{16+36n-43q^2}{192(-1+n)q^2} + \delta_q\frac{32q^2-n(1+34q^2)}{64(-1+n)q^4}, \\ C_3 &= \frac{25}{16} - \frac{-4+q^2}{48(-1+n)q^2} + \delta_q\frac{n+8q^2-10nq^2}{16(-1+n)q^4}, \\ C_4 &= \frac{19}{16} + \frac{4+18n-19q^2}{48(-1+n)q^2} + \delta_q\frac{8q^2-n(1+8q^2)}{16(-1+n)q^4},\end{aligned}$$

$$\begin{aligned}
C_5 &= \frac{65}{48} + \frac{-16+20n^2+44q^2-3n(12+7q^2)}{96(-2+n)(-1+n)q^2} \\
&\quad + \delta_q \frac{-96q^2+n^2(2-56q^2)+3n(-1+54q^2)}{96(-2+n)(-1+n)q^4}, \\
C_6 &= \frac{47}{40} + \frac{8q^2(-10+49q^2)-3nq^2(120+61q^2)+n^2(16+170q^2)}{480(-2+n)(-1+n)q^4} \\
&\quad + \delta_q \frac{-96q^2-2n^2(2+25q^2)+3n(3+50q^2)}{96(-2+n)(-1+n)q^4}, \\
C_7 &= \frac{15q^2(12-59q^2)+10n^3(1+13q^2)+5nq^2(162+137q^2)-12n^2(4+55q^2+11q^4)}{360(-3+n)(-2+n)(-1+n)q^4} \\
&\quad - \delta_q \frac{48q^2-3n(1+26q^2)+n^2(1+26q^2)}{48(-2+n)(-1+n)q^4} + \frac{169}{144}.
\end{aligned}$$

Corollary 4. *The variance of square $CL_2(\mathcal{L}_{n,s})$ is given by (3.2) with the following A_i's, B_j's and C_k's.*

$$\begin{aligned}
A_1 &= \frac{47}{40} + \frac{7+80n^2}{960n^4} - \delta_n \frac{1+16n^2}{64n^4}, \\
A_2 &= \frac{169}{144} + \frac{21+16n+256n^2-4n^3}{2880n^4} - \delta_n \frac{3+4n+52n^2}{192n^4}, \\
B_1 &= \frac{87}{64} + \frac{1}{32n^2} - \delta_n \frac{1+24n^2}{64n^4}, \\
B_2 &= \frac{47}{40} + \frac{4-10n+70n^2-59n^3}{320(-1+n)n^3} + \delta_n \frac{3-4n+72n^2-74n^3}{192(-1+n)n^4}, \\
B_3 &= \frac{65}{48} - \frac{6-10n+n^2}{192(-1+n)n^2} + \delta_n \frac{3+4n+72n^2-82n^3}{192(-1+n)n^4}, \\
B_4 &= \frac{169}{144} + \frac{18-41n+332n^2-264n^3}{1440(-1+n)n^3} + \delta_n \frac{-3+2n-72n^2+115n^3-39n^4}{96(-2+n)(-1+n)n^4}, \\
C_1 &= \frac{19}{12} - \frac{1}{12n^2} - \delta_n \frac{1}{2n^2}, \\
C_2 &= \frac{87}{64} + \frac{16+36n-43n^2}{192(-1+n)n^2} + \delta_n \frac{-1+32n-34n^2}{64(-1+n)n^3}, \\
C_3 &= \frac{25}{16} - \frac{-4+n^2}{48(-1+n)n^2} + \delta_n \frac{1+8n-10n^2}{16(-1+n)n^3}, \\
C_4 &= \frac{19}{16} + \frac{4+18n-19n^2}{48(-1+n)n^2} + \delta_n \frac{-1+8n-8n^2}{16(-1+n)n^3}, \\
C_5 &= \frac{65}{48} + \frac{8+22n-21n^2}{96(-1+n)n^2} - \delta_n \frac{3+94n-162n^2+56n^3}{96(-2+n)(-1+n)n^3}, \\
C_6 &= \frac{47}{40} + \frac{32+196n-183n^2}{480(-1+n)n^2} + \delta_n \frac{9-100n+150n^2-50n^3}{96(-2+n)(-1+n)n^3}, \\
C_7 &= \frac{169}{144} + \frac{22+155n-132n^2}{360(-1+n)n^2} + \delta_n \frac{3-49n+78n^2-26n^3}{48(-2+n)(-1+n)n^3}.
\end{aligned}$$

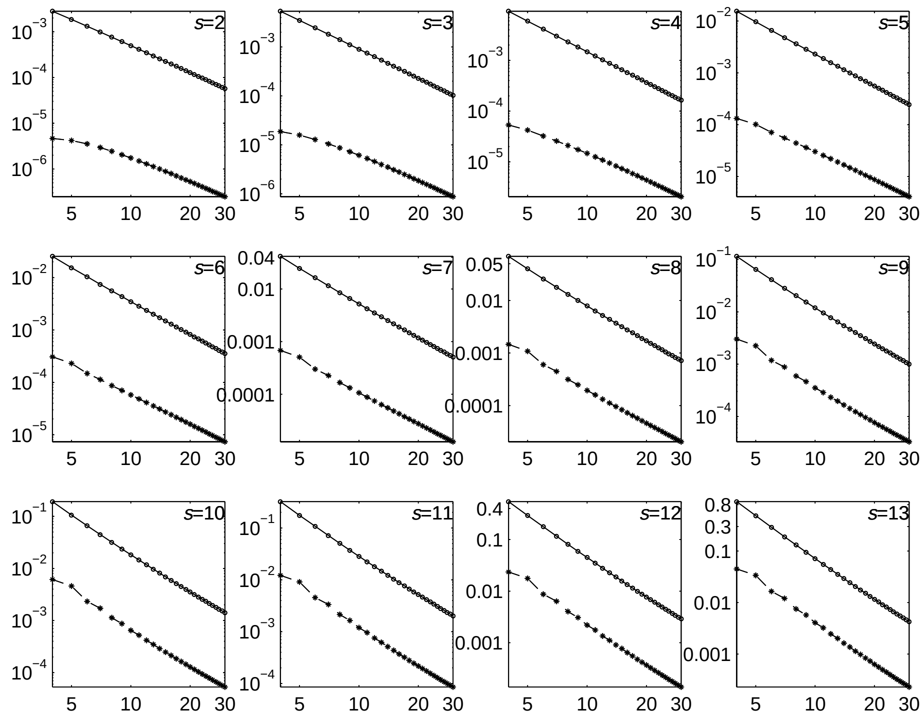

FIGURE 1. Comparison of variance

Formulas (3.1) and (3.2) are too complicated for an intuitive understanding. Therefore, Figure 1 gives numerical comparisons of variance between SRD and LHD $\mathcal{L}_{n,s}$ for $s = 2, \dots, 13$, where "points" is for SRD and "stars" for LHD. The plots show the variance against the number of runs n on a double logarithmic scale. It becomes obvious that LHD $\mathcal{L}_{n,s}$ has much smaller variance of square CL_2 than SRD.

The cases of $s = 2$ and 3 are particularly interesting in practice. For these cases again much simpler formulas can be obtained.

Example 3.2. (a) $s = 2$

$E(CL_2(\mathcal{L}_{n,q^2})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,q^2})^2)$ for q even are

$$\frac{5-34q^2+4q^4+n(-1+26q^2)}{144(-1+n)q^4} \text{ and}$$
$$\frac{(-1+q^2)^2(-225q^4+2n^3(7+2q^2)^2+6n(-4+62q^2+41q^4)-n^2(124+328q^2+79q^4))}{32400(-3+n)(-2+n)(-1+n)^2nq^8},$$

respectively. $E(CL_2(\mathcal{L}_{n,q^2})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,q^2})^2)$ for q odd are

$$\frac{1-68q^2+8q^4+n(7+52q^2)}{288(-1+n)q^4} \text{ and}$$
$$\frac{(-1+q^2)^2(-225q^4+2n^3(7+2q^2)^2+6n(-4+62q^2+41q^4)-n^2(124+328q^2+79q^4))}{32400(-3+n)(-2+n)(-1+n)^2nq^8},$$

respectively.

(b) $s = 2$ and $q = n$
$E(CL_2(\mathcal{L}_{n,2})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,2})^2)$ for n even are

$$\frac{-5-4n+30n^2+4n^3}{144n^4} \quad \text{and} \quad \frac{(-1+n)(1+8n)(2+n-n^2)^2}{32400n^8},$$

respectively. $E(CL_2(\mathcal{L}_{n,2})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,2})^2)$ for n odd are

$$\frac{-1-8n+60n^2+8n^3}{288n^4} \quad \text{and} \quad \frac{(-2+n)^2(1+n)^2(-1-7n+8n^2)}{32400n^8},$$

respectively.
(c) $s = 3$ and $q = n$
$E(CL_2(\mathcal{L}_{n,3})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,3})^2)$ for n even are

$$\frac{29+36n-223n^2-200n^3+663n^4+164n^5}{1728n^6} \quad \text{and}$$
$$\frac{1}{2985984000(-1+n)^2n^{12}}(-6016+3968n-67904n^2+607296n^3-1337752n^4$$
$$-17983064n^5+28836416n^6+19647736n^7-48223786n^8$$
$$+10671771n^9+18977848n^{10}-13190707n^{11}+2610944n^{12}),$$

respectively. $E(CL_2(\mathcal{L}_{n,3})^2)$ and $\mathrm{Var}(CL_2(\mathcal{L}_{n,3})^2)$ for n odd are

$$\frac{-1-46n^2-656n^3+2652n^4+656n^5}{6912n^6} \quad \text{and}$$
$$\frac{(1+n)^2}{2985984000(-2+n)^2n^{12}}(229241+1266861n-3213532n^2$$
$$+19720300n^3-48811906n^4-423698n^5+119671988n^6$$
$$-153693140n^7+86277425n^8-23634483n^9+2610944n^{10}),$$

respectively.

4. Searching uniform designs under CL_2

In this section we discuss the construction of uniform designs and low-discrepancy designs for the centered L_2-discrepancy. When $s = 1$, the following theorem shows that the set of equidistant points is a unique uniform design on $[0, 1]$. This result is consistent with the findings for the star discrepancy [FWa94, Example 1.2].

Theorem 4.1. *When $s = 1$, the unique uniform design on $[0, 1]$ under CL_2 is*

$$\left\{\frac{2i-1}{2n}, i = 1, \ldots, n\right\},$$

and its CL_2^2 is $\frac{1}{12n^2}$.

Proof. Let $\mathcal{P} = \{x_1, x_2, \dots, x_n\}$ be a set in $[0, 1]$. Without loss of generality, we suppose $x_1 \le x_2 \le \cdots \le x_n$ and let $y_k = x_k - 1/2$, $k = 1, 2, \dots, n$.

$$
\begin{aligned}
(CL_2(\mathcal{P}))^2 = {} & \frac{13}{12} - \frac{2}{n}\sum_{k=1}^{n}(1 + \frac{|y_k|}{2} - \frac{|y_k|^2}{2}) \\
& + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}(1 + \frac{|y_k|}{2} + \frac{|y_j|}{2} - \frac{|y_k - y_j|}{2}) \\
= {} & \frac{13}{12} + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}(1 + \frac{|y_k|}{2} + \frac{|y_j|}{2} - \frac{|y_k - y_j|}{2} \\
& -(1 + \frac{|y_k|}{2} - \frac{|y_k|^2}{2}) - (1 + \frac{|y_j|}{2} - \frac{|y_j|^2}{2})) \\
= {} & \frac{1}{12} + \frac{1}{n}(\sum_{k=1}^{n} y_k^2 - \frac{1}{n}\sum_{j>k}(y_k - y_j)) \\
= {} & \frac{1}{12} + \frac{1}{n}\sum_{k=1}^{n}(y_k - \frac{2k-1-n}{2n})^2 - \frac{1}{n}\sum_{k=1}^{n}(\frac{2k-1-n}{2n})^2 \\
= {} & \frac{1}{12n^2} + \frac{1}{n}\sum_{k=1}^{n}(y_k - \frac{2k-1-n}{2n})^2.
\end{aligned}
$$

$(CL_2(\mathcal{P}))^2$ achieves its minimum if and only if $y_k = \frac{2k-1-n}{2n}$, i.e., if and only if $x_k = \frac{2k-1}{2n}$, $k = 1, \dots, n$. The proof is completed. □

Clearly, the solution of (1.7) is not unique when $s > 1$. To search uniform designs for given n and $s (s > 1)$ is probably an NP hard problem when n and s increase. Furthermore, even for moderate values of n and s, it is an almost intractable problem to find a uniform design, because the domain is too large. Therefore, Fang and Hickernell [FH95] suggested considering only a subset of designs, the so-called U-type designs, as the domain for searching uniform designs. U-type designs were defined in Section 1. If one chooses CL_2 as measure of nonuniformity, a design $\boldsymbol{U}^* \in \mathcal{U}_{n,q^s}$ is called U-uniform design, denoted by $U_n(q^s)$, if it has the smallest CL_2-value over $\mathcal{U}_{n,q^s}$.

Figure 2 gives plots of uniform designs and U-uniform designs for $s = 2$ and $n = 2, \dots, 9$. These uniform designs are obtained by the Nelder-Mead simplex method, which in dimension two can be directly applied for $n \le 6$. For $n = 7, 8, 9$,

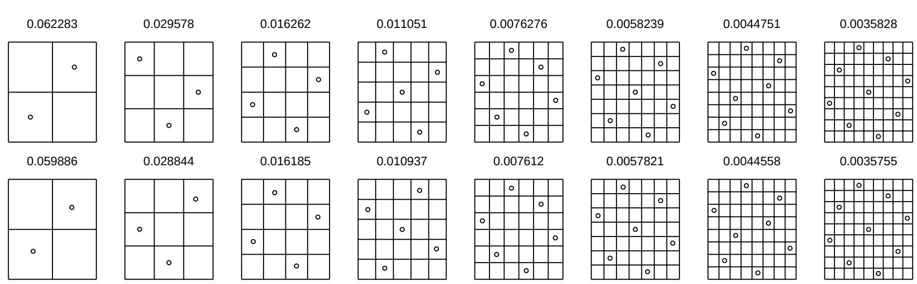

FIGURE 2. Plots of uniform designs and U-uniform designs

the U-uniform designs have to be used as initial values in order to obtain convergence to a low-discrepancy design. Thus, this method is not generally applicable, i.e., for dimension $s > 2$ or large n. The upper plots on Figure 2 are of U-uniform designs and the lower plots are of uniform designs. The CL_2-value of each design is put on the top of its plot. Obviously, U-uniform designs are very close to their corresponding uniform designs. However, when n and s increase, designs obtained by the application of the simplex method often exhibit poor uniformity, while U-uniform designs or U-type designs with low discrepancy can still be obtained. Therefore, we shall construct only U-uniform designs in this paper and call them uniform designs for simplicity throughout the rest of the paper.

Winker and Fang [WF98] applied an implementation of the threshold accepting heuristic to search uniform designs under the discrepancy D defined in (1.4). They found a number of uniform designs and very low-discrepancy designs. In this section, we use a similar implementation for searching uniform designs under CL_2. We also discuss some modifications of the algorithm for improving the results.

As the application of the threshold accepting heuristic to uniform design problems is described in some more detail in [WF97], [FW98], and [WF98], we restrict ourselves to a sketch of the main ideas. Threshold accepting tackles the optimization problem given in (1.7) restricted to U-uniform designs by a refined local search technique. It starts with some arbitrarily chosen U-type design $\mathcal{P} \in \mathcal{U}_{n,q^s}$. Then, in each iteration step the CL_2^2 of the current design is compared with that of some neighbouring design. If the new design is better than the current one, it becomes the new candidate solution. The same holds true if it is not much worse. The threshold up to which a worsening is accepted is defined by the threshold sequence which decreases to zero as the algorithm proceeds (a data driven method for the generation of this threshold sequence is described in [WF97]). If the new design is not accepted based on this criterion, a new trial design is selected in the neighbourhood of the current design.

The final crucial step of the implementation of threshold accepting consists in the definition of neighbourhoods on the set $\mathcal{U}_{n,q^s}$. The approach followed in [WF98] consisted in selecting one or several columns of the induced matrix and exchanging randomly two elements in each of the selected columns. Thus, it is guaranteed that the new candidate design is also a U-type design. A first modification of this neighbourhood concept restricts the exchange within a column to the k next neighbours, i.e., i can be exchanged only with $i-k, \ldots, i+k \mod q$. This restriction was already used in [WF98].

For the purposes of this paper we tested yet another modification, which uses much larger neighbourhoods and is introduced as a ruin-and-recreate approach by [SSSD99]. Instead of exchanging a small number of elements, a complete submatrix of the current design is first eliminated and then reconstructed. The reconstruction step consists in testing all possible permutations of the deleted elements in one column and selecting the permutation which results in the smallest discrepancy together with the unchanged part of the design and the already reconstructed columns. There are still some open questions of how to integrate ruin-and-recreate steps in the most efficient way in the refined local search strategy of threshold accepting. Hence, it is not too surprising that at the current stage this modification rarely outperforms our standard threshold accepting method for the instances analyzed in this section. However, for larger instances, it may exhibit significant improvements which will be assessed in further research.

Given the high complexity of finding uniform designs, in general, it cannot be guaranteed that some threshold accepting implementation will find a uniform design using a reasonable amount of computing resources, although an asymptotic convergence property was proven by [AK91]. Thus, our standard proceeding is to use a limited number of iterations of the algorithm and to assume that the resulting design is a low-discrepancy, if not uniform design. In fact, for the case $s = 2$, where uniform designs under the discrepancy have been obtained by [LF95], our implementation could reproduce these results.

The results on the theoretic expectation and variance of CL_2 for LHD provided in the previous sections allow for an alternative approach. Instead of searching low-discrepancy designs on an absolute scale, we can do so relative to the theoretic expectation and variance. Then, the threshold accepting implementation is run until a design is obtained which has CL_2 lower than the expected value for LHD or lower than the expected value for LHD minus some multiple c of its standard deviation, i.e., $E(CL_2(\mathcal{L}_{n,q^s})^2) - c\sqrt{\mathrm{Var}(CL_2(\mathcal{L}_{n,q^s})^2)}$. The results presented in the next section indicate that c can be chosen from 1 to about 8 as s increases.

Finally, we can contrast the designs optimized with regard to CL_2 with those obtained by [WF98] for the discrepancy.

5. Remarks on new uniform designs

Using the methods described in the previous section, we have obtained a number of low-discrepancy U-type designs under CL_2. Although the modified threshold accepting algorithm is powerful, there can be no guarantee that these designs have minimum CL_2 in the class $\mathcal{U}_{n,q^s}$ or $\mathcal{U}_{n,s}$. Therefore, we have to check whether these designs have low CL_2-value from several angles.

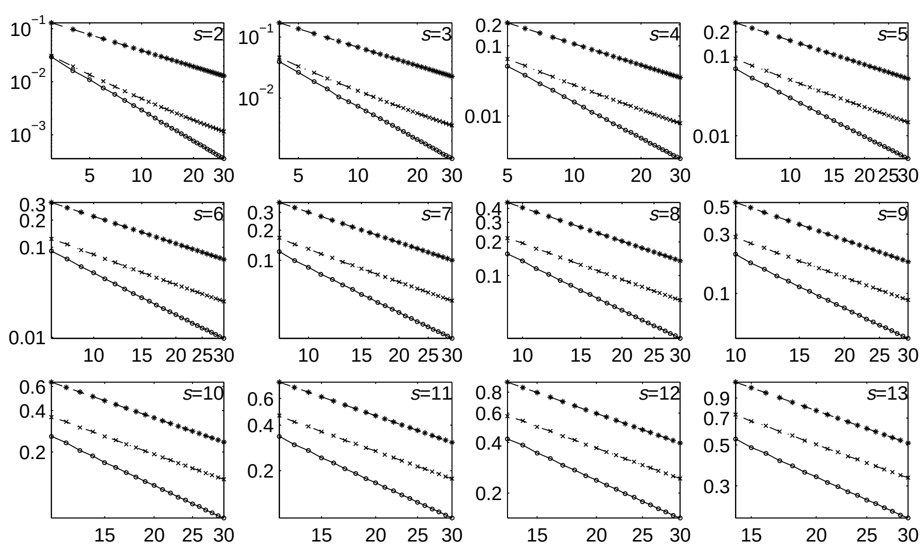

Figure 3. The comparisons among uniform designs by optimization (denoted by point), random designs (by star) and random U-type designs (by x-mark).

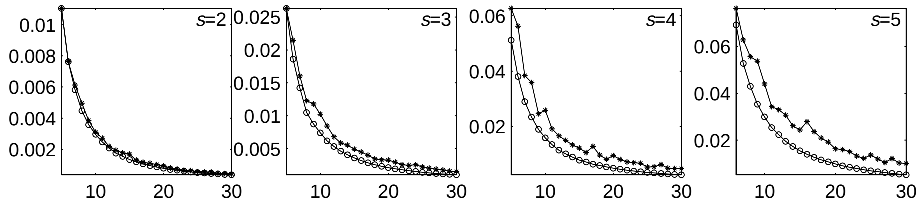

FIGURE 4. Centered L_2 for designs obtained by optimization (circles) and designs from [WF98] (stars)

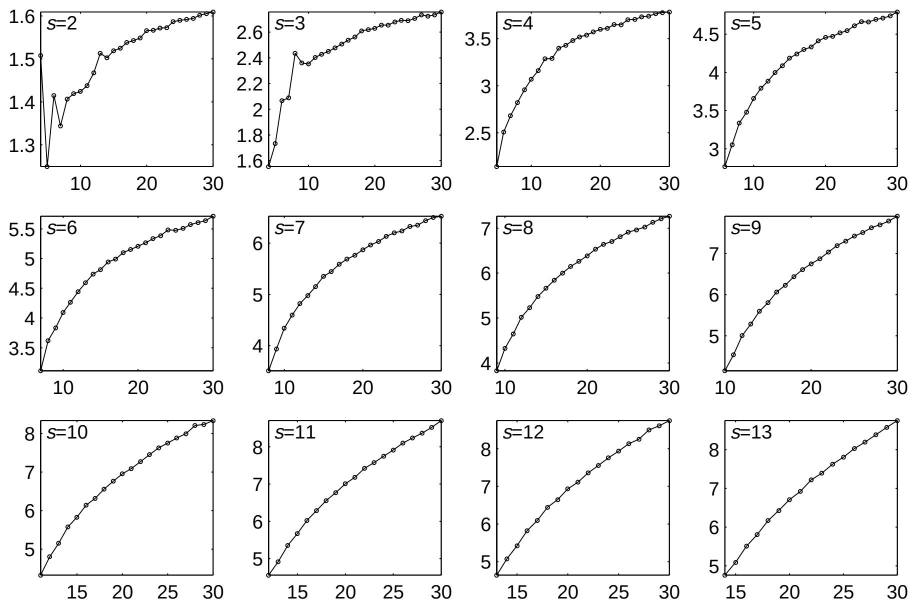

FIGURE 5. The plots of c against n for $s = 2$–13

Firstly, Figure 3 gives plots of $CL_2(\mathcal{P})^2$ against the number of runs n on a double logarithmic scale. The values for the designs obtained by explicit optimization using threshold accepting are marked by a "point"; a "star" denotes the expectation for simple random designs, and an "x-mark" the expectation for Latin hypercube designs. The plots of each design for given s are close to linear lines. The slope of the lines, denoted by $-\beta$, stands for the convergence rate $n^{-\beta}$ of $E(CL_2(\mathcal{P}))$. From Theorem 2.1, the slope of the lines for simple random designs and for Latin hypercube designs should be close to -0.5. The slope of the lines for the optimized U-type designs, which serve as upper bound for the uniform designs, can be estimated by least squares. They vary between -0.9563 and -0.6436 for $2 \leq s \leq 13$. The slope increases as the dimension s increases.

Secondly, when $s = 2$, [LF95] proposed an algorithm by which one can find uniform designs with minimum discrepancy. These designs should also be good designs in the sense of low-CL_2. Figure 4 plots the square CL_2 against n for these designs (stars) and the designs obtained in this paper (circles). It shows that

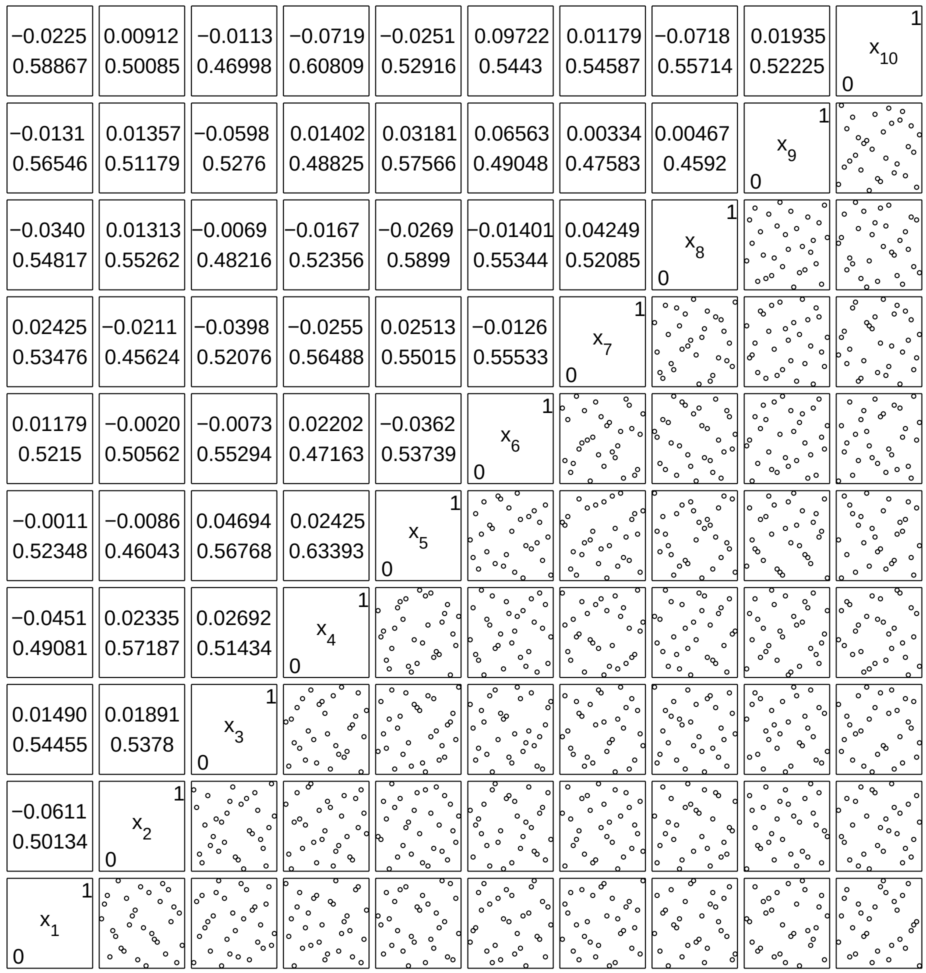

FIGURE 6. Uniform design

the new designs have lower CL_2 than the designs obtained by [LF95]. The same comparison can be performed with regard to the low-discrepancy designs obtained by [WF98], which coincide with the designs of [LF95] in dimension $s = 2$ for $n \leq 23$. The results of the comparison are also shown in Figure 4.

How can we assess the new uniform designs for $s \geq 2$ to have a low CL_2? Let

$$c = \frac{E(CL_2(\mathcal{L}_{n,s}))^2 - (CL_2(\mathcal{P}^*_{n,s}))^2}{\sqrt{\mathrm{Var}((CL_2(\mathcal{L}_{n,s}))^2)}},$$

where $\mathcal{P}^*_{n,s}$ is the new design for given n and s. Figure 5 provides plots of c against n for $s = 2$ to $s = 13$ and $n = s + 1$ to 30. It shows that c increases from 1.25 to 8.75 when n or/and s increase. We find that the distribution of square CL_2 of $\mathcal{L}_{n,s}$ can be approximated by a rescaled beta distribution for given n and s. Then, the results on c in Figure 5 show that the new designs have, in fact, a significantly lower CL_2 than the expectation for LHD.

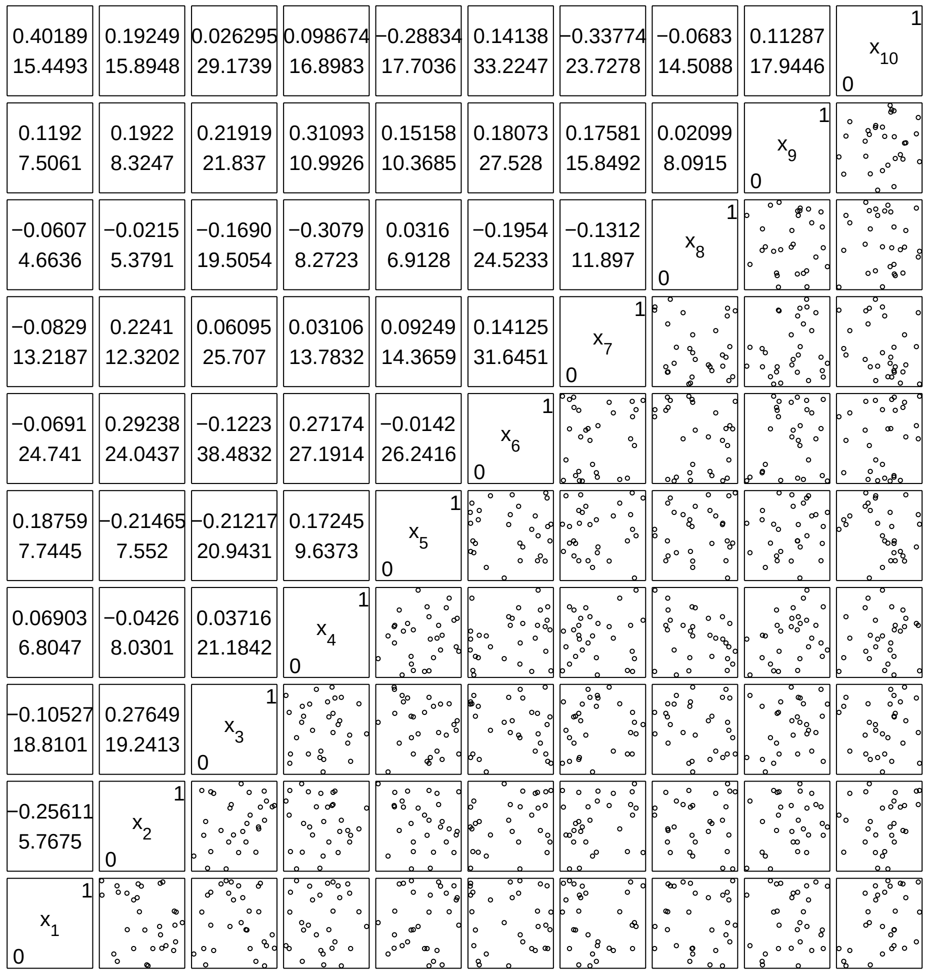

FIGURE 7. Random design

Thirdly, let us look at the projection properties of our new designs. For a uniform design $U_n(q^s)$, we wish that it has good uniformity in all subdimensions, in particular, in all marginal two-dimensional subspaces. For illustration purposes, we choose a new design $U_{30}(30^{10})$ obtained by threshold accepting. Figure 6 gives plots for all marginal two-dimensional subspaces. For each marginal case we list its correlation coefficient and $CL_2^2 * 1000$. The former has been paid much attention by many authors including, e.g., [Owen94]. Similar plots for a simple random design and a Latin hypercube design are given in Figures 7 and 8, respectively. From these plots, the CL_2 values and the correlation coefficients, it becomes clear that the new uniform or low-discrepancy design also has better properties in projection uniformity.

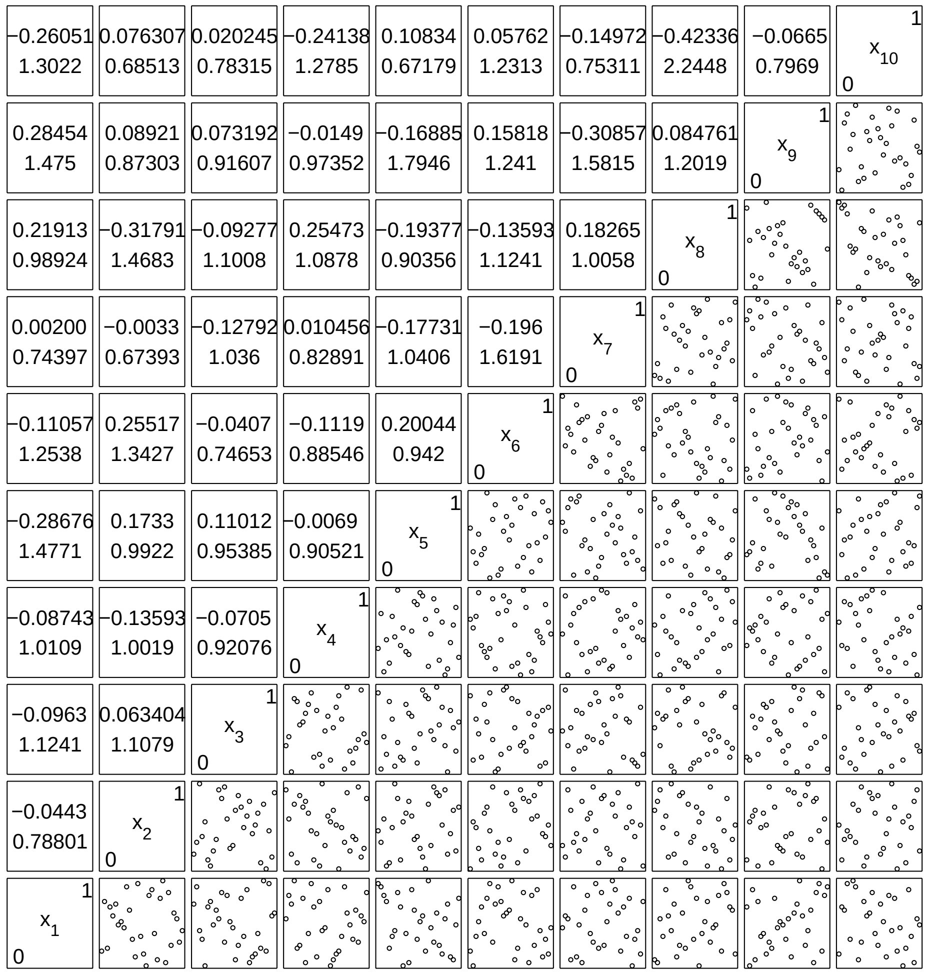

FIGURE 8. A Latin hypercube design randomly chosen

6. Conclusions

In this paper we derived some theoretical results on the expectation and variance of random designs and Latin hypercube designs under the centered L_2-discrepancy (CL_2). It turned out that Latin hypercube designs have a lower expected discrepancy and variance compared to simple random designs. Using these theoretical findings, we proposed an algorithm for the explicit construction of low-discrepancy designs based on a modified version of the global search heuristic threshold accepting. The results indicate that this approach has the potential to generate designs with significantly lower discrepancy than the expectation for Latin hypercube designs.

Further research will aim at extending the numerical results for designs with the number of levels q being smaller than the number of runs n. Also a more detailed analysis of the threshold accepting implementation, in particular with regard to the recent ruin-and-recreate feature may allow for the extension of the approach to larger problem instances.

Appendix

Proof of Theorem 3.1. We prove two cases by the same procedure, but different arguments. For any set $\mathcal{P}$ of n points on C^s the three terms of its CL_2 in (1.6) are denoted by a, b, and c, respectively. Then,

$$E(CL_2(\mathcal{P})^2)^2 = 2aE(CL_2(\mathcal{P}))^2 - a^2 + Eb^2 + 2Ebc + Ec^2$$

and

$$\mathrm{Var}(CL_2(\mathcal{P})^2) = E(CL_2(\mathcal{P})^2)^2 - (E(CL_2(\mathcal{P})^2))^2.$$

Let x, y, z, u be *i.i.d.* uniformly distributed on $[0, 1)$, and let

$$\begin{aligned}
f_1(x) &= 1 + \frac{1}{2}|x - 0.5| - \frac{1}{2}|x - 0.5|^2, \\
g_1(i) &= 1 + \frac{1}{2}|\frac{2i-1-q}{2q}| - \frac{1}{2}|\frac{2i-1-q}{2q}|^2, \\
f_2(x) &= 1 + |x - 0.5|, \\
g_2(i) &= 1 + |\frac{2i-1-q}{2q}|, \\
f_3(x,y) &= 1 + \frac{1}{2}|x - 0.5| + \frac{1}{2}|y - 0.5| - \frac{1}{2}|x - y|, \\
g_3(i,j) &= 1 + \frac{1}{2}|\frac{2i-1-q}{2q}| + \frac{1}{2}|\frac{2j-1-q}{2q}| - |\frac{i-j}{q}|, \\
& \qquad i, j = 1, \ldots, q.
\end{aligned}$$

In the following statement, we use $\stackrel{SRD}{=}$ for random designs and $\stackrel{LHD}{=}$ for Latin hypecube designs $\mathcal{L}_{n,q^s}$.

$$\begin{aligned}
\frac{n^2}{4}E(b^2) &= E(\sum_{k=1}^{n}\sum_{l=1}^{n}\prod_{j=1}^{s} f_1(x_{kj})f_1(x_{lj})) \\
&= \sum_{k=1}^{n}\prod_{j=1}^{s} Ef_1(x_{kj})^2 + 2\sum_{k=1}^{n}\sum_{l=1}^{i-1}\prod_{j=1}^{s} Ef_1(x_{kj})f_1(x_{lj}) \\
&\stackrel{SRD}{=} \sum_{k=1}^{n}(Ef_1(x)^2)^s + 2\sum_{k=1}^{n}\sum_{l=1}^{i-1}(Ef_1(x)f_1(y))^s \\
&\stackrel{LHD}{=} n(\frac{1}{q}\sum_{k=1}^{q} g_1(k)^2)^s + n(n-1)(\sum_{i=1}^{q}\sum_{j=1}^{q} g_1(i)g_1(j)P(i,j))^s,
\end{aligned}$$

and

$$
\begin{aligned}
-\frac{n^3}{2}E(bc) &= E\left(\sum_{k=1}^{n}\sum_{l=1}^{n}\sum_{i=1}^{n}\prod_{j=1}^{s} f_1(x_{kj})f_3(x_{lj},x_{ij})\right)\\
&= \sum_{k=1}^{n}\prod_{j=1}^{s} E(f_1(x_{kj})f_3(x_{kj},x_{kj}))\\
&\quad +2\sum_{k\neq i}^{n}\prod_{j=1}^{s} E(f_1(x_{kj})f_3(x_{kj},x_{ij}))\\
&\quad +\sum_{k\neq i}^{n}\prod_{j=1}^{s} E(f_1(x_{kj})f_3(x_{ij},x_{ij}))\\
&\quad +\sum_{k\neq i\neq l\neq k}^{n}\prod_{j=1}^{s} E(f_1(x_{kj})f_3(x_{lj},x_{ij}))\\
&\overset{SRD}{=} \sum_{k=1}^{n}(E(f_1(x)f_3(x,x)))^s + 2\sum_{k\neq i}^{n}(E(f_1(x)f_3(x,y)))^s\\
&\quad +\sum_{k\neq i}^{n}(E(f_1(x)f_3(y,y)))^s + \sum_{k\neq i\neq l\neq k}^{n}(E(f_1(x)f_3(y,z)))^s\\
&\overset{LHD}{=} n\left(\frac{1}{q}\sum_{k=1}^{q} g_1(k)g_2(k)\right)^s\\
&\quad +2n(n-1)\left(\sum_{i=1}^{q}\sum_{j=1}^{q} g_1(i)g_3(i,j)P(i,j)\right)^s\\
&\quad +n(n-1)\left(\sum_{i=1}^{q}\sum_{j=1}^{q} g_1(i)g_2(j)P(i,j)\right)^s\\
&\quad +n(n-1)(n-2)\left(\sum_{i=1}^{q}\sum_{j=1}^{q}\sum_{l=1}^{q} g_1(i)g_3(j,l)P(i,j,l)\right)^s.
\end{aligned}
$$

Similarly, we have

$$
\begin{aligned}
n^4Ec^2 &\overset{SRD}{=} n(Ef_2(x)^2)^s + 4n(n-1)(Ef_3(x,y)f_2(x))^s\\
&\quad +n(n-1)(Ef_2(x)f_2(y))^s + 2n(n-1)(Ef_3(x,y)^2)^s\\
&\quad +2n(n-1)(n-2)(Ef_2(x)f_3(y,z))^s\\
&\quad +4n(n-1)(n-2)(Ef_3(x,z)f_3(y,z))^s\\
&\quad +n(n-1)(n-2)(n-3)(Ef_3(x,y)f_3(z,u))^s
\end{aligned}
$$

$$
\begin{aligned}
\stackrel{LHD}{=}\quad & n\left(\frac{1}{q}\sum_{k=1}^{q} g_2(k)^2\right)^s \\
&+4n(n-1)\left(\sum_{k=1}^{q}\sum_{j=1}^{q} g_3(k,j)g_2(k)P(k,j)\right)^s \\
&+n(n-1)\left(\sum_{k=1}^{q}\sum_{j=1}^{q} g_2(k)g_2(j)P(k,j)\right)^s \\
&+2n(n-1)\left(\sum_{k=1}^{q}\sum_{j=1}^{q} g_3(k,j)^2P(k,j)\right)^s \\
&+2n(n-1)(n-2)\left(\sum_{k=1}^{q}\sum_{j=1}^{q}\sum_{l=1}^{q} g_2(k)g_3(j,l)P(k,j,l)\right)^s \\
&+4n(n-1)(n-2)\left(\sum_{k=1}^{q}\sum_{j=1}^{q}\sum_{l=1}^{q} g_3(k,l)g_3(j,l)P(k,j,l)\right)^s \\
&+n(n-1)(n-2)(n-3) \\
&\times\left(\sum_{k=1}^{q}\sum_{j=1}^{q}\sum_{l=1}^{q}\sum_{m=1}^{q} g_3(k,j)g_3(l,m)P(k,j,l,m)\right)^s,
\end{aligned}
$$

where $P(k,j)$ is defined in the proof of Theorem 2.1 and $P(k,j,l)$ is the probability that the first three elements of a specific column of the design matrix are k, j, and l, respectively. The notation $P(k,j,l,m)$ can be similarly defined. It is easy to find that

$$
P(i,j,k)=\begin{cases}
\frac{r^3}{n(n-1)(n-2)} & \text{if } i,j,\text{and} k \text{ are not equal to each other,}\\
\frac{r^2(r-1)}{n(n-1)(n-2)} & \text{if } i=j\neq k,\ \text{or } i=k\neq j,\ \text{or } j=k\neq i,\\
\frac{r(r-1)(r-2)}{n(n-1)(n-2)} & \text{if } i=j=k
\end{cases}
$$

and

$$
\begin{aligned}
&P(i,j,k,l)\\
&=\begin{cases}
\frac{r^4}{n(n-1)(n-2)(n-3)} & \text{if } i,j,k, \text{ and } l \text{ are not equal to each other,}\\
\frac{r^3(r-1)}{n(n-1)(n-2)(n-3)} & \text{if only two of } i,j,k, \text{ and } l \text{ are equal to each other,}\\
\frac{r^2(r-1)^2}{n(n-1)(n-2)(n-3)} & \text{if } i=j\neq k=l;\ \text{or } i=k\neq j=l;\ \text{or } i=l\neq j=k,\\
\frac{r^2(r-1)(n-2)}{n(n-1)(n-2)(n-3)} & \text{if only three of } i,j,k, \text{ and } l \text{ are equal to each other,}\\
\frac{r(r-1)(r-2)(r-3)}{n(n-1)(n-2)} & \text{if } i=j=k=l.
\end{cases}
\end{aligned}
$$

The theorem is proved by some straightforward but complicated calculations. □

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Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong; and Chinese Academy of Sciences, Beijing, China
E-mail address: ktfang@math.hkbu.edu.hk

Department of Statistics, Nankai University, Tianjin, China
E-mail address: cxma@nankai.edu.cn

Department of Economics, University of Mannheim, 68131 Mannheim, Germany
E-mail address: Peter.Winker@vwl.uni-mannheim.de