Constructions for Uniform Designs under Wrap-around Discrepancy

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Abstract In this paper, two types of sufficient conditions and lower-bounds for uniform designs under the wrap-around discrepancy are proposed. Based on these results, we can construct uniform designs via combinatorial approach or via computational optimization.

Keywords: uniform designs; wrap-around discrepancy; 1-rotational design; constructions

1 Introduction

Uniform design is a type of "space filling" designs for computer experiments (Bates, et al., 1996). To establish a uniform design one needs to find suitable design points so that they are scattered uniformly on the experimental domain. If we restrict the domain to certain lattice points, then the uniform design is also a fractional factorial design. For a given measure of uniformity M, a uniform design has the smallest M-value over all fractional factorial designs with n runs and m q-level factors. To search a uniform design is an NP hard problem when (n, q, m) increase. Up to now, most of the existing uniform designs are based on the *balanced designs* (or *U-type designs*).

A U-type design $\mathrm{U}(n; q^m)$ denotes a design of n runs and m factors with q levels. This design corresponds to an $n \times m$ matrix $X = (x_1, \cdots, x_m)$ such that each column x_i takes values from a set of q elements, say $\{1, 2, \cdots, q\}$, equally often.

A $\mathrm{U}(n; q^m)$ can be regarded as a set of n points in Q^m, where $Q = \{1, 2, \cdots, q\}$. Thus, a uniform design can be explained as spreading experimental points as evenly as possible over all possible level combinations selected from Q^m. Using a map f: $l \to \frac{2l-1}{2q}$, $l = 1, \cdots, q$, we can also regard a $\mathrm{U}(n, q^m)$ as a set of n points on $\tilde{Q}^m$, where $\tilde{Q} = \{\frac{2l-1}{2q}, l = 1, \cdots, q\}$. Easy to see, the map f is one-one and linear. Throughout the paper, all the $\mathrm{U}(n, q^m)$s are defined on $\tilde{Q}^m$.

As a criterion to measure the degree of uniformity, the star L_p-discrepancy has been widely used in quasi-Monte Carlo methods (or number-theoretic methods) as well as in uniform design theory (see Fang and Wang (1994)). However, as pointed out in Hickernell (1998), the L_p-discrepancy has some weakness. In that paper, Hickernell made some modifications of L_p-discrepancies. The wrap-around L_2 discrepancy (WD_2) is an attractable and interesting one.

The wrap-around discrepancy is defined as follows:

$$(WD_2(\mathcal{P}))^2 = \sum_{u \neq \emptyset} \int_{C^u} \int_{C^u} [\frac{N(\mathcal{P}, J_w(\boldsymbol{x}'_u, \boldsymbol{x}_u))}{n} - Vol(J_w(\boldsymbol{x}'_u, \boldsymbol{x}_u))]^2 d\boldsymbol{x}'_u d\boldsymbol{x}_u,$$

where u is a non-empty subset of the coordinate indices $\{1, 2, \cdots, m\}$, $|u|$ denotes the cardinality of u, C^u is the $|u|$-dimensional unit cube involving the coordinates in u, $N(\mathcal{P} \cap A)$ denotes the number of points of $\mathcal{P}$ falling in A, $\boldsymbol{x}_u$ is the projection of x onto C^u, and

$$J_w(\boldsymbol{x}', \boldsymbol{x}) = \bigotimes_{j=1}^{m} J_w(x'_j, x_j),$$

where $\otimes$ denotes the Kronecher product and

$$J_w(x'_j, x_j) = \begin{cases} [x'_j, x_j), & x'_j \leq x_j; \\ [0, x_j) \cup [x'_j, 1), & x'_j > x_j. \end{cases}$$

An analytical expression of $WD_2(\mathcal{P})$ can be derived.

$$(WD_2(\mathcal{P}))^2 = -(\frac{4}{3})^m + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \prod_{k=1}^{m} \left[\frac{3}{2} - |x_{ik} - x_{jk}|(1 - |x_{ik} - x_{jk}|) \right], \quad (1)$$

where $x_i = (x_{i1}, \cdots, x_{im}) \in \mathcal{P}$. From the definition, we can see that the wrap-around L_p-discrepancy deals with uniformity over the unit cube $\mathcal{P}$ and all the projection of $\mathcal{P}$ over C^u.

In Fang, Ma and Winker (2000) and Fang and Ma (2001), they applied the threshold accepting algorithm to search uniform designs by minimizing discrepancy directly as the objective function. A number of uniform designs or low-discrepancy designs were obtained, which shows that the threshold accepting algorithm is effective in finding uniform designs. However, due to the complication of the discrepancy itself, it is limited to search relatively small designs. In this paper, we will first investigate the analytical expression of the wrap-around discrepancy, then provide sufficient conditions for uniform designs under the wrap-around discrepancy, which not only gives us lower-bounds of a uniform design under the wrap-around discrepancy, but also helps us construct uniform designs or low-discrepancy designs by applying combinatorial approach or by improving the efficiency of the threshold accepting algorithm.

2 Sufficient condition and lower-bound

As Equation (1) shows, the wrap-around discrepancy is only a function of those $|x_{ik} - x_{jk}|(1 - |x_{ik} - x_{jk}|)$s. However, for a U-type design, such values can only be limited into a definite set. Especially, for a U-type design $\mathrm{U}(n; q^m)$, when q is even, these products can only take $\frac{q}{2} + 1$ possible values, i.e., 0, $\frac{2(2q-2)}{4q^2}$, $\frac{4(2q-4)}{4q^2}$, ..., $\frac{q^2}{4q^2}$; when q is odd, these products can only take $\frac{q+1}{2}$ possible values, i.e., 0, $\frac{2(2q-2)}{4q^2}$, $\frac{4(2q-4)}{4q^2}$, ..., $\frac{(q-1)(q+1)}{4q^2}$. Now for any two different rows of the design, i.e., two distinct points $x_i = (x_{i1}, x_{i2}, \ldots, x_{im})$, $x_j = (x_{j1}, x_{j2}, \ldots, x_{jm}) \in \mathcal{P}, i \neq j$, define $\alpha_{ij}^k = |x_{ik} - x_{jk}|(1 - |x_{ik} - x_{jk}|)$, and call them α-values. For a U-type design $\mathrm{U}(n; q^m)$, the number of each different α-value is a constant. Moveover, Simple calculation shows the following table 1.

α − values	number
0	$\frac{mn(n-q)}{2q}$
$\frac{2(2q-2)}{4q^2}$	$\frac{mn^2}{q}$
$\frac{4(2q-4)}{4q^2}$	$\frac{mn^2}{q}$
$\cdots$ $\cdots$	$\cdots$ $\cdots$
$\frac{(q-2)(q+2)}{4q^2}$	$\frac{mn^2}{q}$
$\frac{q^2}{4q^2}$	$\frac{mn^2}{2q}$

α − values	number
0	$\frac{mn(n-q)}{2q}$
$\frac{2(2q-2)}{4q^2}$	$\frac{mn^2}{q}$
$\frac{4(2q-4)}{4q^2}$	$\frac{mn^2}{q}$
$\cdots$ $\cdots$	$\cdots$ $\cdots$
$\frac{(q-3)(q+3)}{4q^2}$	$\frac{mn^2}{q}$
$\frac{(q-1)(q+1)}{4q^2}$	$\frac{mn^2}{q}$

Table 1: left is for q even; right is for q odd.

Different ways of arranging these α-values will result in different wrap-around discrepancies. However, in all cases, the following Theorem states the best arrangement way under the wrap-around discrepancy.

Theorem 2.1 *For a U-type design $U(n; q^m)$, if each pair of two distinct rows contains fixed numbers of different α-values, then it is a uniform design under wrap-around discrepancy. In this case, the wrap-around discrepancy achieves its lower-bound. Define* $\Delta = -(\frac{4}{3})^m + \frac{1}{n}(\frac{3}{2})^m$, *then*

(1) when q is even, the lower-bound is

$$\Delta + \frac{n-1}{2n} \left(\frac{3}{2}\right)^{\frac{m(n-q)}{q(n-1)}} \left(\frac{5}{4}\right)^{\frac{mn}{q(n-1)}} \left(\frac{3}{2} - \frac{2(2q-2)}{4q^2}\right)^{\frac{2mn}{q(n-1)}} \cdots \left(\frac{3}{2} - \frac{(q-2)(q+2)}{4q^2}\right)^{\frac{2mn}{q(n-1)}};$$

(2) when q is odd, the lower-bound is

$$\Delta + \frac{n-1}{2n}\left(\frac{3}{2}\right)^{\frac{m(n-q)}{q(n-1)}}\left(\frac{3}{2}-\frac{2(2q-2)}{4q^2}\right)^{\frac{2mn}{q(n-1)}}\cdots\left(\frac{3}{2}-\frac{(q-1)(q+1)}{4q^2}\right)^{\frac{2mn}{q(n-1)}}.$$

Proof. . According to Equation (1), to minimize $WD_2(\mathcal{P})^2$ is to minimize $\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\prod_{k=1}^{m}\left[\frac{3}{2}-\alpha_{ij}^k\right]$. Since $\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\ln\prod_{k=1}^{m}\left[\frac{3}{2}-\alpha_{ij}^k\right] = \sum_{l=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{m}\ln\left[\frac{3}{2}-\alpha_{ij}^k\right]$ is a constant, we know that when each pair of two distinct rows contains same numbers of different α-values, then for any $1 \le i < j \le n$, $\prod_{k=1}^{m}\left[\frac{3}{2}-\alpha_{ij}^k\right]$ is a constant, which makes $\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\prod_{k=1}^{m}\left[\frac{3}{2}-\alpha_{ij}^k\right]$ achieve its minimum. The expression of the lower-bound of the discrepancy is straightforward according to Table 1. ∎

Notice that when conditions in Theorem 2.1 are satisfied and $q \neq 3$, then m must be a multiple of $n-1$. When these conditions are not satisfied, we can also define the following distance between any two distinct rows i and j:

$$\delta_{ij} = \sum_{k=1}^{m}\ln\left(\frac{3}{2}-\alpha_{ij}^k\right).$$

Theorem 2.2 *For a U-type design $U(n;q^m)$, if the distance between any two distinct rows δ_{ij} is a constant, then it is a uniform design under wrap-around discrepancy. In this case, the wrap-around discrepancy achieves its lower-bound. Define $\Delta = -(\frac{4}{3})^m + \frac{1}{n}(\frac{3}{2})^m$, then*

(1) when q is even, all δ_{ij}s equals the following $\bar{\delta}$

$$\begin{aligned}\bar{\delta} &= \frac{m(n-q)}{q(n-1)}\ln\left(\frac{3}{2}\right)+\frac{mn}{q(n-1)}\ln\left(\frac{5}{4}\right)+\frac{2mn}{q(n-1)}\ln\left(\frac{3}{2}-\frac{2(2q-2)}{4q^2}\right)\\ &\quad+\cdots+\frac{2mn}{q(n-1)}\ln\left(\frac{3}{2}-\frac{(q-2)(q+2)}{4q^2}\right),\end{aligned}$$

and the lower-bound is $\Delta + \frac{n-1}{2n}e^{\bar{\delta}}$;

(2) when q is odd, all δ_{ij}s equals the following $\bar{\delta}$

$$\begin{aligned}\bar{\delta} &= \frac{m(n-q)}{q(n-1)}\ln\left(\frac{3}{2}\right)+\frac{2mn}{q(n-1)}\ln\left(\frac{3}{2}-\frac{2(2q-2)}{4q^2}\right)\\ &\quad+\cdots+\frac{2mn}{q(n-1)}\ln\left(\frac{3}{2}-\frac{(q-1)(q+1)}{4q^2}\right),\end{aligned}$$

and the lower-bound is $\Delta + \frac{n-1}{2n}e^{\bar{\delta}}$.

The proof of Theorem 2.2 is essentially the same as that of Theorem 2.1. In fact, Theorem 2.1 is a special case of Theorem 2.2. However, Theorem 2.1 provides us a direct way for constructing uniform designs under wrap-around discrepancy. For example, if we apply combinatorial approach to construct designs which satisfies the conditions in Theorem 2.1, then we can obtain uniform designs without any computation. While Theorem 2.2 will be helpful for the computational search. Employ the same techniques used in Fang, Lu and Winker (2003), we can accelerate the efficiency of the threshold accepting algorithm. In the next sections, we will discuss some applications of Theorem 2.1 and Theorem 2.2.

3 Construction from resolvable 1-rotational design

In this section, we will construct uniform designs via combinatorial approach. First let us introduce some terminologies in design theorem.

Definition 3.1 *A (v, k, λ) design is an order pair $(V, \mathcal{B})$ which satisfies the following properties:*

1. *V is a set of cardinality v called points;*
2. *$\mathcal{B}$ is a collection of k-subsets of V (called blocks);*
3. *every pair of points of V occurs in exactly λ blocks.*

A (v, k, λ) design $(V, \mathcal{B})$ is 1-rotational if $V = \{\infty\} \cup Z_{v-1}$, and the mapping ϕ from i to $i + 1 \pmod{v-1}$, fixing ∞, is an automorphism of the design. Base blocks for an 1-rotational design are obtained by selecting representatives of the orbits of blocks under the action of ϕ. Denote $\mathcal{P} = \{P_1, P_2, \ldots, P_q\}$ to be a collection of base blocks, if P_1, P_2, $\ldots$, P_q is a partition of V, then the 1-rotational design is said to be resolvable.

Example 3.2 *The following base blocks form a resolvable 1-rotational design* $(12, 3, 2)$*:*

$$\{0, 1, 3\}, \quad \{2, 6, 8\}, \quad \{4, 5, 9\}, \quad \{7, 10, \infty\}.$$

Now given a (v, k, λ) resolvable 1-rotational design, $(V, \mathcal{B})$. Denote $\mathcal{P} = \{P_1, P_2, \ldots, P_q\}$ to be a collection of base blocks, we can construct a U-type design $\mathrm{U}(v; q^{v-1})$ from $(V, \mathcal{B})$ by the following steps.

1. Define a vector of length v, X_1, in such a way that its i-th coordinate $(i \in V)$ has value $w \in \{1, 2, \ldots, q\}$ if and only if point i is contained in the w-th block in $\mathcal{P}$.
2. For each $2 \le k \le v-1$, recursively define X_k in such a way that if the i-th coordinate of X_{k-1} has value w, then the $\phi(i)$-th coordinate of X_k also has value w.
3. Take $X = (X_1^T, X_2^T, \cdots, X_{v-1}^T)$, where X_j^T is the transpose of X_j.

Example 3.3 *The following U-type design $U(12;4^{11})$ is derived from the resolvable 1-rotational design $(12,3,2)$ in Example 3.2:*

row	1	2	3	4	5	6	7	8	9	0	1
0	1	4	3	2	4	2	3	3	1	2	1
1	1	1	4	3	2	4	2	3	3	1	2
2	2	1	1	4	3	2	4	2	3	3	1
3	1	2	1	1	4	3	2	4	2	3	3
4	3	1	2	1	1	4	3	2	4	2	3
5	3	3	1	2	1	1	4	3	2	4	2
6	2	3	3	1	2	1	1	4	3	2	4
7	4	2	3	3	1	2	1	1	4	3	2
8	2	4	2	3	3	1	2	1	1	4	3
9	3	2	4	2	3	3	1	2	1	1	4
10	4	3	2	4	2	3	3	1	2	1	1
∞	4	4	4	4	4	4	4	4	4	4	4

Moreover, for any $1 \leq i,j \leq q$, define a collection $D_{ij} = \{x_i - y_j \pmod{v-1} \mid x_i \in P_i, y_j \in P_j, x_i \neq y_j\}$, and denote $D_s (0 \leq s \leq q-1)$ as the collection of all D_{ij}s with $s \equiv j - i \pmod{q}$. According to the property of a resolvable 1-rotational design, we can easily know that D_0 is a collection of λ copies of $V \backslash \{0\}$ (the difference $-\infty$ is not considered here and after). Further, we have the following Theorem.

Theorem 3.4 *Suppose $(V, \mathcal{B})$ is a (v,k,λ) resolvable 1-rotational design. If for any $1 \leq s \leq \frac{\lfloor q-1 \rfloor}{2}$, the collection of D_s and D_{q-s} is some copies of $V \backslash \{0\}$, then the derived U-type design from $(V, \mathcal{B})$ satisfies the conditions in Theorem 2.1.*

Consider the resolvable 1-rotational design $(12,3,2)$ in Example 3.2, the collection of D_1 and D_3 is six copies of $V \backslash \{0\}$, and D_2 itself is three copies of $V \backslash \{0\}$, so the U-type design $\mathrm{U}(12;4^{11})$ derived in Example 3.3 is a uniform design satisfying the conditions in Theorem 2.1.

Theorem 3.4 states that when we happen to obtain a satisfied resolvable 1-rotational design, then we can construct a desired uniform design without any computation. Although the conditions in Theorem 3.4 may become stronger when the level q is larger, further investigation into the special resolvable 1-rotational designs will be interesting and attractable, especially for modest level q, say, $q = 4$ or 5.

4 The construction by computer search

As stated in Section 1, Threshold Accepting algorithm (TA) has been used in Fang, Ma and Winker (2000) and Fang and Ma (2001) to find uniform designs and low-discrepancy designs. However, in their papers, they use the discrepancy itself as the objective function, which makes the calculation become complex. Here we use the distribution of the run distances, δ_{ij}s, defined in Section 2 as the criterion to search for uniform designs and low-discrepancy designs. Such method can make the computation become much easier. According to Theorem 2.2, we know that when the distance between any two distinct rows δ_{ij} is a constant, then the design is a uniform design under wrap-around discrepancy. So the aim of our computational optimization is to adjust these δ_{ij}s as equally as possible.

Since the threshold accepting algorithm has been discussed extensively in many papers, here we only list the main steps.

The algorithm is started with a randomly generated U-type design D_0. Afterwards, in each iteration the algorithm tries to replace the current solution D_c with a new one. The new design D_n is generated in a given neighborhood of the current solution. In fact, it is a small perturbation of the current solution. The distribution of the run distances δ_{ij}s is calculated for the new design and the result is compared with that of the current design. If the result is better, or is worse but within our threshold limit, then we replace the current solution with the new one. As with Wang and Fang (1998), the aim of using a temporary worsening up to a given threshold value is to avoid getting stuck into a local minimum.

The implementation of the algorithm to the approximation of uniform designs should take into account several aspects.

Firstly, the definition of local neighborhoods. Obviously, in each iteration of the algorithm, the new solution D_n should still be a U-type design. This requirement can be easily fulfilled by selecting one column of the current solution D_c and exchanging two elements in the selected column. Further modifications can be implemented in this approach. For example, more than one columns can be chosen to exchange the elements. And the same way can be performed by exchanging more than two elements in the selected columns. If the algorithm is implemented in the parallel way, then the neighborhood concept can restrict the exchange within a column to the s (s is a factor of the number of runs n) cliques.

Secondly, the objective function. In each iteration, the discrepancy difference between the new and the current design $\Delta = WD_2(D_n) - WD_2(D_c)$ must be calculated. However, For a single exchange of two elements in the selected column, there are altogether $2(n-2)$ δ_{ij}s updated. Thus instead of evaluating the wrap-around discrepancy in (1) again, we need only recalculate the $2(n-2)$ differences of $e^{\delta_{ij}}$ for those δ_{ij} updated. As discussed in Fang, Lu and Winker (2003), when we change the objective function from the discrepancy difference between the two designs to some updates of δ_{ij}s, we are hoped to dramatically improve the performance of the algorithm. Moveover, Theorem 2.2 also gives us a hint that the wrap-around discrepancy of a design will be smaller as all δ_{ij}s become closer to $\bar{\delta}$. So we can assign a weight to each δ_{ij} according to its departure from $\bar{\delta}$. Those considerably large or relatively small δ_{ij}s are supposed to have more changes to be updated. When the design scale is large, this improvement is also hoped to make sense to the effectivity of the algorithm.

Finally, parameters. During the implementation of the threshold accepting algorithm, we also need to define a threshold sequence τ_r, $r = 1, \ldots, n_R$ and the number of iterations for each τ_r. Details for determination of these parameters can refer to Winker (2001), we do not get much further here.

The implementation of this optimization approach will be carried out in the next research.

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