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Constructing uniform designs under mixture discrepancy

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ABSTRACT

The discrepancies have played an important role in quasi-Monte Carlo methods and uniform design. Zhou et al. (2013) proposed a new type of discrepancy, mixture discrepancy (MD), and showed that MD may be a better uniformity measure than wrap-around L_2-discrepancy and centered L_2-discrepancy. In this paper, some constructing methods for uniform designs under MD are shown. The relationship between MD and the generalized wordlength pattern for multi-level design is given, then the level permutation technique is shown as a useful tool to search uniform designs. Moreover, it is shown that MD can be represented by quadratic form and the global optimum solution of experimental design under MD is also given. Furthermore, by such quadratic form, the relationship between a design and its complementary design is shown, which can be used to construct uniform design with large size.

1. Introduction

As a type of space-filling design, uniform design has been widely applied in manufacturing, system engineering, pharmaceutics, and natural sciences, see Fang and Wang (1994) and Fang et al. (2006). The main idea of uniform design is to scatter its design points to be uniformly on the experimental domain under some uniformity measure. In the literature, the star discrepancy proposed by Weyl (1916), centered L_2-discrepancy (CD) and the wrap-around L_2-discrepancy (WD) proposed by Hickernell (1998a,b) are popularly used as uniformity measures. For assessing the property of different discrepancies, Fang et al. (2006) proposed seven criteria such as invariant under permuting factors and/or runs, invariant under the coordinates rotation, measuring projection uniformity, have some geometric meaning, easy to compute, satisfying Koksma–Hlawka inequality and consistent with other criteria in experimental designs. The CD and the WD satisfy the seven criteria, and the star discrepancy only satisfies part of them. Moreover, Zhou et al. (2013) proposed two additional criteria to assess the property of different discrepancies, i.e., sensitivity on a shift for one or more dimensions and no curse of dimensionality. It was shown that the CD has a significant dimensionality effect, then the CD is not suitable for assessing the uniformity of designs especially when the number of factors is large. Moreover, the WD has a shortcoming of sensitivity on a shift for one or more dimensions. Zhou et al. (2013) also introduced a new type of uniformity measure, mixture discrepancy (MD), which satisfies all of the nine aforementioned criteria. Then, the MD may be a more reasonable uniformity measure than the CD and the WD.

In this paper, the MD is considered as the uniformity measure for constructing uniform designs. Zhou et al. (2013) showed the relationship between the MD and the popular used criterion in fractional factorial design, generalized wordlength

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pattern (GWP, see Xu and Wu, 2001), for two-level design. It is worth to show the relationship for multi-level cases, since this relationship is helpful to search uniform designs. As shown in Zhou and Xu (2014), a generalized minimum aberration design usually has low discrepancy. Moreover, Zhou et al. (2012) used the quadratic form of WD to search uniform design under WD, Jiang and Ai (2014) also considered the quadratic form for CD, WD and other types of discrepancy to construct uniform designs without replications. In this paper, the quadratic form of MD is also given, then based on this quadratic form some theoretic results are shown to be used to search uniform designs.

The remainder of this paper is organized as follows: Section 2 introduces the definition of mixture discrepancy and the relationship between MD and GWP, then some examples show that the level permutation technique can be used to search designs with lower MD than that of generalized minimum aberration designs. Section 3 gives the quadratic form of MD. Based on such quadratic form, the global optimum solution under MD is shown, and the relationship between the MD of any design and the MD of its complementary design is also shown, which is useful to construct uniform design with large size. Some concluding remarks are given in Section 4.

2. Mixture discrepancy

Let $U(n; q_1, \ldots, q_s)$ be a n-run asymmetrical design with s factors each having respectively $q_1, \ldots, q_s$ levels. Then $U(n; q_1, \ldots, q_s)$ is an $n \times s$ design matrix whose ith column has elements $1, \ldots, q_i$, $i = 1, \ldots, s$. When all q_i's are equal to q, the design is called *symmetrical* and denoted by $U(n; q^s)$. Let $\mathcal{U}(n; q_1, \ldots, q_s)$ and $\mathcal{U}(n; q^s)$ be the sets of all $U(n; q_1, \ldots, q_s)$ and $U(n; q^s)$, respectively. For any design $\boldsymbol{X} = (u_{ij}) \in \mathcal{U}(n; q_1, \ldots, q_s)$, denote its reduced design be $\tilde{\boldsymbol{X}} = (x_{ij})$ with $x_{ij} = (u_{ij} - 0.5)/q_j$, then $\tilde{\boldsymbol{X}} \subset C^s = [0, 1]^s$. Let the (squared) mixture discrepancy of $\boldsymbol{X}$ be same as that of $\tilde{\boldsymbol{X}}$, i.e., (see Zhou et al., 2013)

$$\mathrm{MD}(\boldsymbol{X}) = \left(\frac{19}{12}\right)^s - \frac{2}{n}\sum_{i=1}^{n}\prod_{j=1}^{s}\left(\frac{5}{3} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right|^2\right)$$
$$+ \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\prod_{j=1}^{s}\left(\frac{15}{8} - \frac{1}{4}\left|x_{ij} - \frac{1}{2}\right| - \frac{1}{4}\left|x_{kj} - \frac{1}{2}\right| - \frac{3}{4}|x_{ij} - x_{kj}| + \frac{1}{2}|x_{ij} - x_{kj}|^2\right). \quad (1)$$

Under MD a uniform design $U(n; q_1, \ldots, q_s)$ has the minimum MD over $\mathcal{U}(n; q_1, \ldots, q_s)$.

Now consider the relationship between MD and GWP, which can be used to obtain nearly uniform design. For a design $\boldsymbol{X} \in \mathcal{U}(n; q^s)$, consider an ANOVA model $Z = Y_0\alpha_0 + Y_1\alpha_1 + \cdots + Y_s\alpha_s + \epsilon$, where Z is the vector of n observations, α_0 is the intercept and Y_0 is an $n \times 1$ vector of 1's, α_j is the vector of all j-factor interactions and Y_j is the matrix of orthonormal contrast coefficients for α_j, and ϵ is the random error. Define $A_j(\boldsymbol{X}) = N^{-2}\|Y_0^T Y_j\|^2$, $j = 0, \ldots, s$, where $\|Y\|^2 = \sum_{i,j} y_{ij}^2$ for a matrix $Y = (y_{ij})$. It is obvious that $A_0(\boldsymbol{X}) = 1$. The vector $(A_1(\boldsymbol{X}), A_2(\boldsymbol{X}), \ldots, A_s(\boldsymbol{X}))$ is called the generalized wordlength pattern of design $\boldsymbol{X}$. The generalized minimum aberration (GMA) criterion is to sequentially minimize $A_1(\boldsymbol{X}), A_2(\boldsymbol{X}), \ldots, A_s(\boldsymbol{X})$.

For every factor of the design $\boldsymbol{X} \in \mathcal{U}(n; q^s)$, the level permutation is defined by $\{1, \ldots, q\} \to \{\pi_1, \ldots, \pi_q\}$, where $\{\pi_1, \ldots, \pi_q\}$ is a permutation of $\{1, \ldots, q\}$. When considering all $q!$ possible level permutations for every factor, we obtain $(q!)^s$ combinatorially isomorphic designs of $\boldsymbol{X}$. Denote the set of these designs as $\mathcal{P}(\boldsymbol{X})$, and the mean of mixture discrepancies of all the designs in $\mathcal{P}(\boldsymbol{X})$ be $\overline{\mathrm{MD}}(\boldsymbol{X})$, i.e., $\overline{\mathrm{MD}}(\boldsymbol{X}) = \frac{1}{(q!)^s}\sum_{D \in \mathcal{P}(\boldsymbol{X})} \mathrm{MD}(D)$. Zhou et al. (2013) showed that the mixture discrepancy was also defined by the tool of reproducing kernel Hilbert space and its kernel function is $\mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) = \prod_{i=1}^{s} f(x_i, y_i)$, where $f(x, y) = 15/8 - |x - 0.5|/4 - |y - 0.5|/4 - 3|x - y|/4 + |x - y|^2/2$. Then, $f(x, y) \geq 0$ and $f(x, x) + f(y, y) > f(x, y) + f(y, x)$ for any $x \neq y$, $x, y \in [0, 1]$, i.e., $f(x, y)$ satisfies the conditions in Lemma 1 of Zhou and Xu (2014), which showed that the mean of mixture discrepancies $\overline{\mathrm{MD}}(\boldsymbol{X})$ can be expressed by the linear combination of the GWP of the design $\boldsymbol{X}$. Then we have the following result.

Theorem 1. *For a design $\boldsymbol{X} \in \mathcal{U}(n; q^s)$, the mean MD, $\overline{MD}(\boldsymbol{X})$, can be expressed by the linear combination of the GWP of the design $\boldsymbol{X}$:*

$$\overline{MD}(\boldsymbol{X}) = \left(\frac{19}{12}\right)^s - 2\left(\frac{19q^2+1}{12q^2}\right)^s + \left(\frac{38q^2+7}{24q^2}\right)^s \sum_{i=0}^{s}\left(\frac{4q+4}{38q^2+7}\right)^i A_i(\boldsymbol{X}),$$

when q is odd and

$$\overline{MD}(\boldsymbol{X}) = \left(\frac{19}{12}\right)^s - 2\left(\frac{76q^2+1}{48q^2}\right)^s + \left(\frac{19q^2+2}{12q^2}\right)^s \sum_{i=0}^{s}\left(\frac{2q+2}{19q^2+2}\right)^i A_i(\boldsymbol{X}),$$

when q is even.

The proof of Theorem 1 can be obtained from the Lemma 1 of Zhou and Xu (2014) and we omit it. It should be mentioned that when $q = 2$, the level permutation does not change the uniformity of designs, then $\overline{\mathrm{MD}}(\boldsymbol{X}) = \mathrm{MD}(\boldsymbol{X})$ and Theorem 1 is an extension of Theorem 3 of Zhou et al. (2013), which only considers the relationship between the MD and GWP for