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Mixture discrepancy for quasi-random point sets

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ABSTRACT

There are various discrepancies that are measures of uniformity for a set of points on the unit hypercube. The discrepancies have played an important role in quasi-Monte Carlo methods. Each discrepancy has its own characteristic and some weakness. In this paper we point out some unreasonable phenomena associated with the commonly used discrepancies in the literature such as the L_p-star discrepancy, the center L_2-discrepancy (CD) and the wrap-around L_2-discrepancy (WD). Then, a new discrepancy, called the mixture discrepancy (MD), is proposed. As shown in this paper, the mixture discrepancy is more reasonable than CD and WD for measuring the uniformity from different aspects such as the intuitive view, the uniformity of subdimension projection, the curse of dimensionality and the geometric property of the kernel function. Moreover, the relationships between MD and other design criteria such as the balance pattern and generalized wordlength pattern are also given.

1. Introduction

Quasi-Monte Carlo methods (QMCM) have been widely used in multivariate numerical integration, numerical simulation, experimental design and statistical inference (see [5,8,11]). QMCM were motivated by multidimensional numerical integration. Suppose that one wants to find a multidimensional integral

$$I(g) = \int_{C^s} g(\boldsymbol{x}) d\boldsymbol{x}$$

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by using the sample mean,

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

where $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is a set of points on $C^s = [0, 1]^s$. The Koksma–Hlawka (K–H) inequality shows that

$$|I - \hat{I}(\mathcal{P})| \leq V(g)D(\mathcal{P}), \tag{2}$$

where $D(\mathcal{P})$ is the star discrepancy of $\mathcal{P}$ not depending on g and $V(g)$ is the total variation of the function g in the sense of Hardy and Krause (see [8]). As a measure of uniformity for a set on C^s, the star discrepancy proposed by Weyl [13] has been widely used in the past ninety years. The K–H inequality suggests choosing a set of points having the lowest star discrepancy. The key idea of QMCM is to generate a set of n points, denoted by $\mathcal{P}$, on the unit cube $\mathbf{C}^s$ for given (n, s) such that $D(\mathcal{P})$ is minimized, or at least the discrepancy is lower in a certain sense. Denote by $F(\boldsymbol{x})$ the distribution function of the uniform distribution on C^s and by $F_n(\boldsymbol{x})$ the empirical distribution of $\mathcal{P}$. The star discrepancy is defined by

$$D(\mathcal{P}) = \max_{\boldsymbol{x}\in C^s} |F_n(\boldsymbol{x}) - F(\boldsymbol{x})|. \tag{3}$$

The so-called Kolmogorov–Smirnov statistic for the goodness-of-fit test is the first application of the star discrepancy to statistics. Unfortunately, the computational complexity for calculating $D(\mathcal{P})$ increases exponentially as n and/or s increase. An extension of the star discrepancy is the L_p-star discrepancy defined by

$$D_p(\mathcal{P}) = \left[\int_{C^s} |F_n(\boldsymbol{x}) - F(\boldsymbol{x})|^p d\boldsymbol{x}\right]^{1/p}, \quad \text{or}$$

$$D_p(\mathcal{P})^p = \int_{C^s} \left|\frac{N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))}{n} - \mathrm{Vol}([\mathbf{0}, \boldsymbol{x}))\right|^p d\boldsymbol{x}, \tag{4}$$

where $[\mathbf{0}, \boldsymbol{x}) = [0, x_1) \times \cdots \times [0, x_s)$, $N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))$ denotes the number of points of $\mathcal{P}$ falling in $[\mathbf{0}, \boldsymbol{x})$, and $\mathrm{Vol}(A)$ represents the volume of A. The star discrepancy is the case of L_∞-star discrepancy. For when $p = 2$, Warnock [12] gave an analytic formula for calculating the L_2-star discrepancy. The computational complexity of the L_2-star discrepancy is about $O(n^2)$ and is reasonable. Unfortunately, the L_p-star discrepancy ($p \neq \infty$) exhibits some disadvantages: it suffers from projection uniformity over all subdimensions and sometimes it implies some unreasonable results. Furthermore, the L_p-star discrepancy does not have the property of reflection invariance, i.e., it is not invariant under rotating coordinates of the points as the origin $\mathbf{0}$ plays a special role. To overcome these disadvantages, Hickernell [6,7] used the tool of the reproducing kernel Hilbert space to propose several modifications of the L_p-star discrepancy. Among them, the centered L_2-discrepancy (CD) and the warp-around L_2-discrepancy (WD) have nice properties, such as invariance under reordering the runs, relabeling coordinates and coordinate shift. The CD and WD count the projection uniformity and satisfy the K–H inequality.

These two discrepancies have played an important role in experimental design. Fang et al. [1] proposed several criteria for assessing measures of uniformity for construction of experimental designs as follows:

[C_1] Are invariant under permuting factors and/or runs.

[C_2] Are invariant under coordinate rotation.

[C_3] Measure not only uniformity of $\mathcal{P}$ on C^s, but also projection uniformity of $\mathcal{P}$ on C^u, where u is a non-empty subset of $\{1, \ldots, s\}$.

[C_4] Have some geometric meaning.

[C_5] Are easy to compute.

[C_6] Satisfy K–H inequality.

[C_7] Are consistent with other criteria in experimental design.