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A survey of high-discrepancy sequences

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Abstract. This article surveys recent results and open questions on high-discrepancy sequences.

Keywords. discrepancy, high-discrepancy sequences, Kolmogorov superposition integrals, Owen's scrambling, (t, m, d) -nets, (t, d) -sequences

1. INTRODUCTION

First, we introduce the definition of discrepancy [7, 14]. For a point set $P_N = \{X_0, X_1, \dots, X_{N-1}\}$ of N points in $[0, 1]^d$ and an interval $J \subseteq [0, 1]^d$, we define $A_N(J)$ as the number of n , $0 \leq n \leq N-1$, with $X_n \in J$ and $\mu(J)$ is the volume of J . Then the discrepancy of P_N is defined by

$$D_d(P_N) = \sup_J \left| \frac{A_N(J)}{N} - \mu(J) \right|,$$

where the supremum is taken over all intervals J of the form

$$J = \prod_{i=1}^d [\alpha_i, \beta_i), \text{ for } 0 \leq \alpha_i < \beta_i \leq 1. \quad (1)$$

The uniform distribution of an infinite sequence $X_0, X_1, \dots \in [0, 1]^d$ is defined as follows [7, 14]: If an infinite sequence of points X_n , $n = 0, 1, \dots$, in $[0, 1]^d$ satisfies that for any interval J in (1),

$$\lim_{N \rightarrow \infty} \frac{A_N(J)}{N} = \mu(J),$$

then we say that the sequence is uniformly distributed in $[0, 1]^d$. It is known that a sequence is uniformly distributed if and only if $\lim_{N \rightarrow \infty} D_d(P_N) = 0$. An important application of uniformly distributed sequences is numerical integration due to the well-known Koksma-Hlawka theorem, which is given as

$$\left| \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(X_n) \right| \leq D_d(P_N) V(f),$$

where $V(f)$ is the variation of the function $f(x)$ in the sense of Hardy and Krause [7, 8, 13, 20]. Also it is known [5] that the integral of any Riemann integrable function is equal to the limit of the arithmetic mean of function values at sample points if and only if the sequence of sample points is uniformly distributed.

High-discrepancy sequences are defined as those sequences which are not uniformly distributed, in other

words, the discrepancy $D_d(P_N)$ does not converge to zero as N goes to infinity. In this survey, we focus on a sequence of points in $[0, 1]^d$ ($d \geq 2$) which are distributed only on the diagonal line between $(0, \dots, 0)$ and $(1, \dots, 1)$. It is obvious that such a sequence is far from uniformly distributed, namely a high-discrepancy sequence. In the case of high discrepancy sequences, the Koksma-Hlawka theorem is of no use because the discrepancy $D_d(P_N)$ does not converge to zero. In this article, however, we show that there are several classes of functions for which the fast convergence of numerical integration can be guaranteed by the use of high-discrepancy sequences.

2. HIGH-DISCREPANCY SEQUENCES ON THE DIAGONAL LINE

In this section, we discuss two cases. The first case is that a sequence of points are uniformly distributed on the diagonal line between $(0, \dots, 0)$ and $(1, \dots, 1)$. Secondly, we consider the non-uniform case.

2.1. UNIFORM CASE

First, we need recall some necessary definitions from the net theory [2, 7, 14]. An elementary interval in base b ($b \geq 2$) is a subinterval of $[0, 1]^d$ of the form

$$E = \prod_{i=1}^d [a_i b^{-k_i}, (a_i + 1) b^{-k_i}), \quad (0 \leq a_i < b^{k_i}, k_i \geq 0).$$

A (t, m, d) -net in base b is a point set of b^m points in $[0, 1]^d$ such that $A(E, b^m) = b^t$ for every elementary interval E in base b , with $V(E) = b^{t-m}$ ($0 \leq t \leq m$). A (t, d) -sequence in base b is an infinite sequence, $X = (X_n)_{n \geq 0}$, of points in $[0, 1]^d$ such that for all $h \geq 0$ and $m > t$, the point set $\{[X_{hb^m}]_{b,m}, \dots, [X_{(h+1)b^m-1}]_{b,m}\}$ is a (t, m, d) -net, where $[X_n]_{b,m}$ denotes the coordinate-wise b -ary m -digit truncation of a point X_n .

The practical construction of (t, m, d) -nets and (t, d) -sequences is based on the so-called *generator matrices* over

$GF(b)$, where the base b is assumed to be a prime power (for more detail of their definition and relevant information, see [2, 7, 14]). Hereafter, we denote by \mathfrak{S}_d a class of (t, d) -sequences in base two whose generator matrices are nonsingular and lower-triangular. Note that this class includes high-discrepancy sequences uniformly distributed on the diagonal line between $(0, \dots, 0)$ and $(1, \dots, 1)$ which corresponds to (t, d) -sequences in base two whose generator matrices are all identical.

The Walsh functions are defined by

$$\text{wal}(0, x) = 1, \text{ for } x \in [0, 1),$$

and for an integer $k \geq 1$,

$$\text{wal}(k, x) = (-1)^{\sum_{j=1}^{\infty} b_{j-1} a_j} = (-1)^{(\mathbf{k}, X)}$$

where $k = b_0 + b_1 2 + \dots$, and $x = a_1 2^{-1} + a_2 2^{-2} + \dots$ in the binary expansion, and $\mathbf{k} = (b_0, b_1, \dots)$ and $X = (a_1, a_2, \dots)$ are the binary vector representation of k and x , respectively. Then, we have the following theorem [16]:

Theorem 1. An L_2 function on $[0, 1]^d$ can be written as

$$f(x_1, \dots, x_d) = \sum_{k_1, \dots, k_d \geq 0} c_{k_1, \dots, k_d} \text{wal}(k_1, x_1) \cdots \text{wal}(k_d, x_d).$$

We have

$$\begin{aligned} I(f) &:= \int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \cdots dx_d \\ &= 2^{d-1} \left(\int_{[0, \frac{1}{2}]^d} f(x_1, \dots, x_d) dx_1 \cdots dx_d \right. \\ &\quad \left. + \int_{[\frac{1}{2}, 1]^d} f(x_1, \dots, x_d) dx_1 \cdots dx_d \right) - \Delta_d, \end{aligned}$$

where

$$\Delta_d = \sum_{\substack{0 \leq k_1, \dots, k_d \leq 1 \\ (k_1, \dots, k_d) \neq (0, \dots, 0) \\ k_1 + \dots + k_d = 0 \pmod{2}}} c_{k_1, \dots, k_d}.$$

We now consider a class of functions for which $\Delta_d = 0$. First, we give some definitions.

Definition 1. Let $m \geq 1$ be an integer and let u be a nonempty subset $\{j_1, \dots, j_{|u|}\} \subseteq \{1, \dots, d\}$. We define

$$\phi_{u,m}(x_1, \dots, x_d) = \prod_{i=1}^{|u|} \text{wal}(k_{j_i}^{(m)}, x_{j_i}),$$

for $2^{m-1} \leq k_{j_1}^{(m)}, \dots, k_{j_{|u|}}^{(m)} < 2^m$.

Definition 2. A function class \mathfrak{F}_d consists of functions

$$f(x_1, \dots, x_d) = c_0 + \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} c_{u,m} \phi_{u,m}(x_1, \dots, x_d),$$

where c_0 and $c_{u,m}$, $m = 1, 2, \dots$, are constants satisfying

$$|c_0| + \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} |c_{u,m}| 2^{m-1} \leq M < \infty.$$

Here, M is a constant.

We have the following results [15, 16]:

Theorem 2. For any function $f(x_1, \dots, x_d)$ in \mathfrak{F}_d , we have $\Delta_d = 0$.

Theorem 3. For any sequence X_n , $n = 0, 1, \dots$, in the class \mathfrak{S}_d , the integration error e_N of any function f in \mathfrak{F}_d is given by

$$\begin{aligned} e_N(X_n, f) &:= \left| I(f) - \frac{1}{N} \sum_{n=0}^{N-1} f(X_n) \right| \\ &< \frac{1}{N} \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} |c_{u,m}| \min(2^{m-1}, N) \\ &< \frac{M}{N}, \end{aligned}$$

where the last inequality follows from Definition 2.

An important consequence from the above result is that the ‘‘low-discrepancy’’ approach is not the only way for accelerating the computation of high dimensional numerical integration. If one considers a class of functions for which the uniform distribution is not a necessary condition for the integral of any function in the class to be equal to the limit of the arithmetic mean of function values, there is a possibility to develop faster algorithms based on the ‘‘high-discrepancy’’ approach than simple Monte Carlo and/or ‘‘low-discrepancy’’ methods.

2.1.1. OWEN’S SCRAMBLING

Owen’s scrambling scheme is described as follows [9, 10]: Let $b \geq 2$ be an integer. Assume that σ is a mapping from the interval $[0, 1)$ onto itself. A b -ary scrambling is a mapping σ from the b -ary representation of $A \in [0, 1)$ to the b -ary representation of $\sigma(A) \in [0, 1)$ determined in the following way: Let $A = a_1 b^{-1} + a_2 b^{-2} + \dots$, where a_1, a_2, \dots are in $\{0, 1, \dots, b-1\}$. Then the first b -ary digit of $\sigma(A)$ is $\pi(a_1)$, where π is a fixed permutation of the set $\{0, 1, \dots, b-1\}$. Next, for each possible value of a_1 , we fix a permutation π_{a_1} of $\{0, 1, \dots, b-1\}$, and define the second b -ary digit as $\pi_{a_1}(a_2)$. We can continue with the definitions of the third digit, fourth digit, and so on, in the same way, and obtain $\pi_{a_1, a_2}(a_3), \pi_{a_1, a_2, a_3}(a_4), \dots$. In this scrambling scheme, each permutation is uniformly distributed over the $b!$ possible permutations and the permutations are mutually independent. In d dimensions, we consider an d -tuple of b -ary scramblings $(\sigma_1, \dots, \sigma_d)$. Owen showed that if $\sigma_1, \dots, \sigma_d$ are chosen as fully random and mutually independent, then the d -dimensional scrambling preserves the t -values of (t, m, d) -nets and (t, d) -sequences.

Owen also analyzed the variance of the integration error for his scrambling. His formula for the variance of the integration error holds for any L_2 function on $[0, 1]^d$. We need recall the definition of gain coefficients $\Gamma_{u,\kappa}$ introduced in [10]. Denote a set of N points in $[0, 1]^d$ by $X_n = (X_n^{(1)}, \dots, X_n^{(d)})$, $n = 0, \dots, N-1$. The gain coefficient

cient is defined by

$$\Gamma_{u,\kappa} = \frac{1}{N(b-1)^{|u|}} \sum_{n=0}^{N-1} \sum_{n'=0}^{N-1} \prod_{i \in u} \left(b 1_{\lfloor b^{k_i+1} X_n^{(i)} \rfloor = \lfloor b^{k_i+1} X_{n'}^{(i)} \rfloor} - 1 1_{\lfloor b^{k_i} X_n^{(i)} \rfloor = \lfloor b^{k_i} X_{n'}^{(i)} \rfloor} \right),$$

where $\kappa = (k_1, \dots, k_d)$. Then, we have the following formula for the variance of the integration error in terms of Owen's scrambling:

$$\begin{aligned} V(f; N; X_n) &= \mathbb{E} \left[\left(\frac{1}{N} \sum_{n=0}^{N-1} f(X_n) - I(f) \right)^2 \right] \\ &= \frac{1}{N} \sum_{u \neq \emptyset} \sum_{\kappa} \Gamma_{u,\kappa} \sigma_{u,\kappa}^2, \end{aligned}$$

where $\sigma_{u,\kappa}^2$ is the variance of the step function, which is defined from the b -ary Haar wavelet expansion of $f(x_1, \dots, x_d)$ (for the detail, see [9, 10]). We should note that the variance for simple Monte Carlo methods with N samples is

$$\frac{\sigma^2(f)}{N} = \frac{1}{N} \sum_{u \neq \emptyset} \sum_{\kappa} \sigma_{u,\kappa}^2. \quad (2)$$

Now, we consider an application of Owen's scrambling to d -dimensional high-discrepancy points which consist of d copies of a $(0, m, 1)$ -net in base b , that is to say, all d coordinates of the point set are identical to a $(0, m, 1)$ -net in base b . As we said before, for some class of functions "low-discrepancy" is not a necessary condition for the speed-up of their numerical integration. We proved the following theorem [17]:

Theorem 4. Denote $k_{\max} = \max_{i \in u} k_i$, and denote by $h(u, \kappa)$ the number of i such that $k_i = k_{\max}$. For Owen's scrambling of high-discrepancy points, which consist of d copies of a $(0, m, 1)$ -net in base b , if $k_{\max} < m$, then the gain coefficient is given by

$$\Gamma_{u,\kappa} = b^{\ell(u,\kappa)} \left(1 - \frac{1}{(1-b)^{h(u,\kappa)-1}} \right), \quad (3)$$

where $\ell(u, \kappa) = m - k_{\max} - 1$, and if $k_{\max} \geq m$, then $\Gamma_{u,\kappa} = 1$.

In the particular case of $b = 2$, the equation (3) becomes much simpler, i.e.,

$$\Gamma_{u,\kappa} = \begin{cases} 0 & \text{if } h(u, \kappa) \text{ is odd,} \\ 2^{\ell(u,\kappa)+1} & \text{otherwise.} \end{cases}$$

By taking into account the equation (2), we obtain a necessary and sufficient condition for scrambled high-discrepancy points to have smaller variance than simple Monte Carlo methods as follows:

Corollary 1. For the integration of a L_2 function on $[0, 1]^d$, scrambled high-discrepancy points in base b have

smaller variance than simple Monte Carlo methods if and only if

$$\sum_{u \neq \emptyset} \sum_{\kappa} \left(b^{\ell(u,\kappa)} \left(1 - \frac{1}{(1-b)^{h(u,\kappa)-1}} \right) - 1 \right) \sigma_{u,\kappa}^2 < 0, \quad (4)$$

where the number of samples is $N = b^m$.

In the particular case of $b = 2$, the inequality (4) becomes much simpler, i.e.,

$$\sum_{u \neq \emptyset} \sum_{\kappa_e} (2^{\ell(u,\kappa_e)+1} - 1) \sigma_{u,\kappa_e}^2 < \sum_{u \neq \emptyset} \sum_{\kappa_o} \sigma_{u,\kappa_o}^2,$$

where the number of samples is $N = 2^m$ and κ_e or κ_o is such κ that $h(u, \kappa)$ is even or odd, respectively. Interestingly enough, for the class of functions \mathfrak{F}_d in Definition 2, we have $\sigma_{u,\kappa_e} = 0$ for all u and κ_e and $\sigma_{u,\kappa_o} \neq 0$ for some u and κ_o , in other words, scrambled high-discrepancy points in base two give smaller variance than simple Monte Carlo methods.

2.2. NON-UNIFORM CASE

Kolmogorov superposition theorem tells us that for any integer $d \geq 1$, any continuous function $f(x_1, \dots, x_d)$ on $[0, 1]^d$ can be represented as a superposition of one-dimensional functions, i.e.,

$$f(x_1, \dots, x_d) = \sum_{q=0}^{2d} g_q \left(\sum_{i=1}^d a_i \Psi_q(x_i) \right), \quad (5)$$

where $g_q(x)$, $q = 0, 1, \dots, 2d$, are continuous functions determined depending on $f(x_1, \dots, x_d)$, and a_i , $i = 1, \dots, d$ are constants with $\sum_{i=1}^d a_i = 1$, determined independently of $f(x_1, \dots, x_d)$. And $\Psi_q(x)$, $q = 0, 1, \dots, 2d$, are monotone increasing and continuous function on $[0, 1]$, determined independently of $f(x_1, \dots, x_d)$. How to construct these functions and constants can be found in [1], which also includes more detail and latest information on this theorem.

Based on this theorem, we introduced a Kolmogorov superposition integral as follows [18]:

Definition 3. A Kolmogorov superposition integral is defined by

$$I_d(g; \Psi) := \int_{[0,1]^d} g \left(\sum_{i=1}^d a_i \Psi(x_i) \right) dx_1 \cdots dx_d,$$

where $\Psi(x)$ is any monotone increasing function on $[0, 1]$ which is continuous in $(0, 1)$, and a_1, \dots, a_d are constants with $\sum_{i=1}^d a_i = 1$. And $g(x)$ is any continuous function such that $|I_d(g; \Psi)| < \infty$. We remark that $\Psi(x)$ can be $\pm\infty$ at the ends of the unit interval $[0, 1]$.

A practical example of Kolmogorov superposition integral is given below.

Example 1. According to Papageorgiou [12], many finance problems can be written as Kolmogorov superpo-

sition integrals with

$$\begin{aligned} g(x) &= \max(a \exp(bx) - K, 0), \\ \Psi(x) &= \phi^{-1}(x), \\ a_1 = \dots = a_d &= 1/d, \end{aligned}$$

where a and b are appropriate constants.

We also introduced a Kolmogorov superposition high-discrepancy sequence [18].

Definition 4. A Kolmogorov superposition high-discrepancy sequence is defined as a sequence of points

$$X_n = (s_n, \dots, s_n) \in [0, 1]^d, \quad n = 0, 1, 2, \dots,$$

with $s_n = \Psi^{-1}(p^{-1}(v_n))$, where $p(x)$ is the distribution function corresponding to $\sum_{i=1}^d a_i \Psi(x_i)$, and $v_n, n = 0, 1, 2, \dots$, is a one-dimensional low-discrepancy sequence.

The function $p(x)$ can be obtained either by repeatedly calculating the convolution of $\Psi(x)$ or by using the products of the characteristic function of the probability distribution function $\Psi(x)$. As the definition makes clear, Kolmogorov superposition high-discrepancy sequences are distributed only on the diagonal line between $(0, \dots, 0)$ and $(1, \dots, 1)$. We should note that the sequence is constructed independently of $g(x)$, the integrand of Kolmogorov superposition integrals. On the integration error, we obtained the following theorem [11, 18]:

Theorem 5. Denote $\rho(x) = g(p^{-1}(x))$. For a Kolmogorov superposition integral, if the function $\rho(x)$ is of bounded variation, then the error of the numerical integration using a Kolmogorov superposition high-discrepancy sequence is given by $O((\log N)/N)$, where N is the number of points.

We remark that the function $\rho(x)$ associated with the integral described in Example 1 is not of bounded variation. However, the results of Papageorgiou [12] imply that the integration error for the high-discrepancy sequence is $O(N^{-1+o(1)})$, where the asymptotic constant is independent of d .

2.2.1. SOFTWARE IMPLEMENTATION

We give the software implementation of Kolmogorov superposition high-discrepancy sequences (KS-HDS) as follows:

[Preprocessing] By using the parameters, $d, p(x)$, and $\Psi(x)$, compute KS-HDS as

$$X_n = (s_n, \dots, s_n) \in [0, 1]^d, \quad n = 0, 1, 2, \dots,$$

with $s_n = \Psi^{-1}(p^{-1}(v_n))$, where $v_n, n = 0, 1, 2, \dots$, is the van der Corput sequence. Then store it in the memory.

[Main processing] Once the integrand $g(x)$ is given, call N points of the KS-HDS from the memory, and compute

$$\frac{1}{N} \sum_{n=0}^{N-1} g(\Psi(s_n))$$

as an approximation to the integral.

3. DISCUSSIONS

As in the Braun-Griebel implementation of Kolmogorov superposition theorem [1], when the dimension d goes to infinity, all the functions $\Psi_q(x), q = 0, 1, \dots, 2d$, become identical to $\Psi_0(x)$. Therefore, we can use the same high-discrepancy sequence for all $g_q(x), q = 0, 1, \dots, 2d$ in (5). Namely, the integration of any continuous function $f(x_1, \dots, x_d)$ over $[0, 1]^d$,

$$I(f) = \sum_{q=0}^{2d} I_d(g_q; \Psi_q) \approx \sum_{q=0}^{2d} I_d(g_q; \Psi_0)$$

can be computed by using the high-discrepancy sequence, X_0, X_1, \dots , described in Definition 4 with $\Psi_0(x)$ provided that the dimension is large enough. We point out that in this case it is not necessary to know the decompositions $g_q(x), q = 0, 1, \dots, 2d$, explicitly, because we can apply the sequence, X_0, X_1, \dots , directly to the function $f(x_1, \dots, x_d)$, that is to say,

$$I(f) = \int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \cdots dx_d \approx \frac{1}{N} \sum_{n=0}^{N-1} f(X_n).$$

This fact can be regarded as the blessing of dimensionality discussed by Donoho [3]. However, it is open to determine how large the dimension should be to replace the $\Psi_q(x), q = 0, 1, \dots, 2d$, by a single function.

The optimal discrepancy is defined as follows:

$$D_{d,N}^{\text{opt}} = \inf_{P_N} D_d(P_N),$$

where the infimum is taken over all sets of N points in $[0, 1]^d$. Hinrichs [4] proved the following lower bound:

$$D_{d,N}^{\text{opt}} \geq \min(\epsilon, cd/N),$$

where $0 < c < 1$ and $\epsilon > 0$ are absolute constants. We stress that under the constraint $N \leq d$, the discrepancy $D_{d,N}^{\text{opt}}$ never converges to zero as N goes to infinity. This implies that under the constraint $N \leq d$, a sequence of points can not be uniformly distributed in $[0, 1]^d$, in other words, it becomes a high-discrepancy sequence.

Thus, we now present the following conjecture:

Conjecture 1. For any $N \geq 2$ and $d \geq N$, there exists a set of N points on the diagonal line between $(0, \dots, 0)$ and $(1, \dots, 1)$ in $[0, 1]^d$ such that its discrepancy is optimal.

At present, the conjecture was confirmed only for the case $N = 2$ with any $d \geq 2$ [6, 19]. It is interesting to prove or disprove it for general case $N \geq 3$ and $d \geq N$.

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