HIGH-DISCREPANCY SEQUENCES

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Abstract. First, it is pointed out that the uniform distribution of points in $[0, 1]^d$ is not always a necessary condition for every function in a proper subset of the class of all Riemann integrable functions to have the arithmetic mean of function values at the points converging to its integral over $[0, 1]^d$ as the number of points goes to infinity. We introduce a formal definition of the d -dimensional *high-discrepancy sequences*, which are not uniformly distributed in $[0, 1]^d$, and present motivation for the application of these sequences to high-dimensional numerical integration. Then, we prove that there exist non-uniform (∞, d) -sequences which provide the convergence rate $O(N^{-1})$ for the integration of a certain class of d -dimensional Walsh function series, where N is the number of points.

1. Introduction

It is well known [3] that the uniform distribution of points $X_n, n = 0, 1, \dots$, in $[0, 1]^d$ is a necessary and sufficient condition for every function $f(x_1, \dots, x_d)$ in the class of all Riemann integrable functions over $[0, 1]^d$, hereafter denoted by $\mathfrak{R}_d$, to satisfy

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

It is also known [3] that for the class of all continuous functions over $[0, 1]^d$, which is a proper subset of $\mathfrak{R}_d$, the uniform distribution is a necessary and sufficient condition for every function in the class to satisfy equation (1). The well-known

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Koksma–Hlawka theorem implies that the class of all functions over $[0, 1]^d$ of bounded variation in the sense of Hardy and Krause is another proper subset of $\mathfrak{R}_d$ for which the uniform distribution is also a necessary and sufficient condition for every function in the class to satisfy equation (1).

However, little is known about what happens to any other proper subsets of $\mathfrak{R}_d$. Although the uniform distribution of sample points is a sufficient condition for every function in any proper subset of $\mathfrak{R}_d$ to satisfy equation (1), it is not always a necessary condition. The purpose of this paper is to explore a possibility to develop faster algorithms for a proper subset of $\mathfrak{R}_d$ based on non-uniform sample points than Monte Carlo and/or quasi-Monte Carlo methods. In the next section, we first introduce a formal definition of the d -dimensional *high-discrepancy sequences*, which are not uniformly distributed in $[0, 1]^d$, and present motivation for the application of these sequences to high-dimensional numerical integration. Then, we prove that there exist non-uniform (∞, d) -sequences which provide the convergence rate $O(N^{-1})$ for the integration of a certain class of d -dimensional Walsh function series, where N is the number of points. In the last section, we discuss the significance of this result and future research directions.

2. Main result

2.1. Discrepancy and (t, d) -sequences

For a point set $P_N = \{X_0, X_1, \dots, X_{N-1}\}$ of N points in $I^d = [0, 1]^d$ and a subinterval J of I^d , we define $A(J, N)$ as the number of n , $0 \leq n \leq N-1$, with $X_n \in J$ and $V(J)$ is the volume of J . Then the discrepancy of P_N is defined by

$$D_N^{(d)} = \sup_J \left| \frac{A(J, N)}{N} - V(J) \right|,$$

where the supremum is taken over all subintervals J of the form $\prod_{i=1}^d [0, y_i)$. For more mathematical detail on discrepancy, see, e.g., [1, 4–7].

An elementary interval in base b ($b \geq 2$) is a subinterval of I^d of the form

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

A (t, m, d) -net in base b is a point set of b^m points in I^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 I^d such that for

all $h \geq 0$ and $m > t$, the point set $\{[X_{hb^m}]_m, \dots, [X_{(h+1)b^m-1}]_m\}$ is a (t, m, d) -net, where $[X_n]_m$ denotes the coordinate-wise m -digit truncation of a point X_n .

The general construction principle of (t, d) -sequences in base b is as follows:

- (i) R is a commutative ring with $\text{card}(R) = b$ and $B = \{0, 1, \dots, b-1\}$;
- (ii) for an integer $r \geq 1$, choose bijections ψ_r from B to R with $\psi_r(0) = 0$ for all sufficiently large r ;
- (iii) for integers i, j such that $1 \leq i \leq d$ and $j \geq 1$, choose bijections $\lambda_{i,j}$ from R to B ;
- (iv) for integers i, j, r as above, choose elements $c_{j,r}^{(i)} \in R$.

If $n = \sum_{r=1}^{\infty} a_r(n)b^{r-1}$ is the b -ary expansion of $n \geq 0$, set $X_n^{(i)} = \sum_{j=1}^{\infty} x_{n,j}^{(i)}b^{-j}$, where $x_{n,j}^{(i)} = \lambda_{i,j}(\sum_{r=1}^{\infty} c_{j,r}^{(i)}\psi_r(a_r(n)))$ for $1 \leq i \leq d$. Here, the matrices $C^{(i)} = (c_{j,r}^{(i)})_{j \geq 1, r \geq 1}$ are called the generator matrices of X . Then, the sequence $X = (X_n)_{n \geq 0}$, with coordinates $X_n^{(i)}$ as above, becomes a (t, d) -sequence in base b , where the value of t is determined by the linear independence structure of generator matrices. Hereafter, we assume that b is a prime power, and that R in the construction principle is the finite field $GF(b)$. Let

$$\mathbf{c}_\ell^{(i)}(m) = (c_{\ell,1}^{(i)}, \dots, c_{\ell,m}^{(i)}) \in GF(b)^m,$$

and let

$$C(k_1, \dots, k_d; m) = \{\mathbf{c}_\ell^{(i)}(m) \mid 1 \leq \ell \leq k_i, 1 \leq i \leq d\}.$$

Define $\rho(C; m)$ as the maximal integer K such that $C(k_1, \dots, k_d; m)$ is linearly independent over $GF(b)$ for all non-negative integers $k_1, \dots, k_d$ satisfying $\sum_{1 \leq i \leq d} k_i = K$. We have the following result [5, 7].

PROPOSITION 1. *If an integer $t \geq 0$ satisfies $t \geq m - \rho(C; m)$ for each integer $m > t$, then the sequence defined in the above becomes a (t, d) -sequence in base b .*

2.2. Definition and motivation for high-discrepancy sequences

First, we introduce the definition of high-discrepancy sequences.

Definition 1. If a sequence of points $X_n, n = 0, 1, \dots$, in $[0, 1]^d$ satisfies that for all $N > 1$, the discrepancy $D_N^{(d)}$ of the first N points is given by

$$D_N^{(d)} = O(1), \tag{2}$$

then we call it a *high-discrepancy sequence*, where the implied constant in the O notation depends only on the dimension d .

We should note that if the right-hand side in equation (2) is replaced by $O((\log N)^d/N)$, then it is the definition of a low-discrepancy sequence. High-discrepancy sequences are those sequences which are not uniformly distributed, and *vice versa*. We have the following proposition.

PROPOSITION 2. *A (t, d) -sequence in base two for which the first rows of its generator matrices are all identical to $(1, 0, 0, \dots)$ is a high-discrepancy sequence.*

Proof. From Proposition 1, the sequence is an (∞, d) -sequence, i.e. a (t, d) -sequence with t being infinity. Since it is distributed in only two sub-domains, $[0, 1/2]^d$ and $[1/2, 1]^d$, the proof follows. $\square$

Note that there are two types of (∞, d) -sequences, i.e. uniform or non-uniform. The sequence introduced in Proposition 2 is a non-uniform (∞, d) -sequence.

We give the following theorem, which motivates us to investigate the application of high-discrepancy sequences defined in the above to high-dimensional numerical integration.

THEOREM 1. *If an L_2 function in d dimensions is written as*

$$f(x_1, \dots, x_d) = \sum_{k_1, \dots, k_d \geq 0} c_{k_1, \dots, k_d} \cos(2\pi k_1 x_1) \cdots \cos(2\pi k_d x_d),$$

then we have

$$\begin{aligned} \int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d \\ = 2^{d-1} \left(\int_{[0,1/2]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d \right. \\ \left. + \int_{[1/2,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d \right). \end{aligned} \quad (3)$$

Proof. Since

$$\int_0^1 \cos(2\pi kx) dx = 0$$

for any $k \geq 1$, we have

$$\int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = c_{0, \dots, 0}.$$

Since

$$\int_0^{1/2} \cos(2\pi kx) dx = \int_{1/2}^1 \cos(2\pi kx) dx = 0$$

for any $k \geq 1$, we have

$$\int_{[0,1/2]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{c_{0,\dots,0}}{2^d},$$

and

$$\int_{[1/2,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{c_{0,\dots,0}}{2^d}.$$

Thus, the proof is complete. $\square$

We can also consider the following type of L_2 functions in d dimensions:

$$f(x_1, \dots, x_d) = c_0 + \sum_{k_1, \dots, k_d \geq 1} c_{k_1, \dots, k_d} \sin(2\pi k_1 x_1) \cdots \sin(2\pi k_d x_d).$$

It is easy to see that if the dimension d is odd, this class of functions also satisfy equation (3). Recently, Tezuka and Papageorgiou [9] showed that there exists an exact cubature with only one point for this class of functions in any d dimensions.

In what follows, we show that there exist non-uniform (∞, d) -sequences which provide the convergence rate $O(N^{-1})$ for the integration of a class of d -dimensional Walsh function series.

2.3. A class of d -dimensional Walsh function series

The Walsh functions are defined by

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

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 $k = b_0 + b_1 2 + \dots$, $x = a_1 2^{-1} + a_2 2^{-2} + \dots$ 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.

THEOREM 2. *A function in the d -dimensional L_2 space 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

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

where

$$\Delta_d = \sum_{\substack{0 \leq k_1, \dots, k_d \leq 1 \\ (k_1, \dots, k_d) \neq (0, \dots, 0) \\ k_1 + \dots + k_d \equiv 0 \pmod{2}}} c_{k_1, \dots, k_d}. \quad (4)$$

Proof. First, we have

$$\int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = c_{0, \dots, 0}.$$

Since

$$\int_0^{1/2} \text{wal}(1, x) dx = - \int_{1/2}^1 \text{wal}(1, x) dx = \frac{1}{2},$$

and

$$\int_0^{1/2} \text{wal}(k, x) dx = \int_{1/2}^1 \text{wal}(k, x) dx = 0$$

for any $k \geq 2$, we have

$$\int_{[0,1/2]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{1}{2^d} \sum_{0 \leq k_1, \dots, k_d \leq 1} c_{k_1, \dots, k_d},$$

and

$$\int_{[1/2,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{1}{2^d} \sum_{0 \leq k_1, \dots, k_d \leq 1} (-1)^{k_1 + \dots + k_d} c_{k_1, \dots, k_d}.$$

Thus, the proof is complete. $\square$

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

Definition 2. Let $m \geq 1$ be an integer and let u be a non-empty 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 3. We define a class $\mathfrak{F}_d$ which 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 theorem.

THEOREM 3. For any function $f(x_1, \dots, x_d)$ in $\mathfrak{F}_d$, we have

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

Proof. From equation (4) and Definition 3, it follows that the quantity Δ_d in Theorem 2 becomes zero for the case of $\mathfrak{F}_d$. Thus, the proof is complete. $\square$

2.4. Convergence rate for the high-dimensional integration

Hereafter, we denote by $\mathfrak{S}_d$ a class of (t, d) -sequences in base two whose generator matrices are non-singular and lower-triangular. Note that this class is a special subset of the class of non-uniform (∞, d) -sequences introduced in Proposition 2. We prove the following theorem.

THEOREM 4. For any sequence $\mathbf{s}_n, n = 0, 1, \dots$, in the class $\mathfrak{S}_d$, the integration error e_N of any function f in $\mathfrak{F}_d$ is given by

$$e_N(\mathbf{s}_n, f) := \left| I(f) - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{s}_n) \right| < \frac{1}{N} \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} |c_{u,m}| \min(2^{m-1}, N).$$

From the condition in Definition 3, we have $e_N(\mathbf{s}_n, f) = O(N^{-1})$, where the asymptotic constant is M . In order to prove the above theorem, we need the following three lemmas, which are generalizations of Lemmas 2, 3 and 4 in [8]. Let $s_n, n = 0, 1, \dots$, be a sequence in $\mathfrak{S}_1$, and let $s_{n,m}$ denote the m th bit of s_n .

LEMMA 1. Suppose that $m \geq 1$. For all $n = h \cdot 2^m, h = 0, 1, \dots$, and for all $0 \leq \ell < 2^{m-1}$, we have

$$s_{n+\ell, m} = 1 - s_{n+\ell+2^{m-1}, m}.$$

Proof. If we compare $n+\ell$ and $n+\ell+2^{m-1}$, only the coefficient of 2^{m-1} in their binary representation is different while all of the others are identical. Since the generator matrix is non-singular and lower-triangular, this completes the proof. $\square$

LEMMA 2. Suppose that $m \geq 1$. For all $n = h \cdot 2^m, h = 0, 1, \dots$, and for all $0 \leq \ell < 2^{m-1}$, we have

$$\text{wal}(k, s_{n+\ell}) = -\text{wal}(k, s_{n+\ell+2^{m-1}}),$$

where k is any integer with $2^{m-1} \leq k < 2^m$.

Proof. Since the generator matrix is non-singular and lower-triangular, we have $s_{n+\ell, e} = s_{n+\ell+2^{m-1}, e}$ for all $1 \leq e < m$. From the assumption that $k = b_0 + b_1 2 + \dots + b_{m-1} 2^{m-1}$ with $b_{m-1} = 1$ and Lemma 1, the proof is complete. $\square$

For d dimensions, we denote a sequence in $\mathfrak{S}_d$ by $\mathbf{s}_n = (s_n^{(1)}, \dots, s_n^{(d)}), n = 0, 1, \dots$. Then we have the following lemmas.

LEMMA 3. Suppose that $m \geq 1$. Let u be any non-empty subset $\{j_1, \dots, j_{|u|}\} \subseteq \{1, \dots, d\}$. If the cardinality $|u|$ is odd, then for all $n = h \cdot 2^m, h = 0, 1, \dots$, and for all $0 \leq \ell < 2^{m-1}$, we have

$$\phi_{u,m}(\mathbf{s}_{n+\ell}) = -\phi_{u,m}(\mathbf{s}_{n+\ell+2^{m-1}}).$$

Proof. Denote

$$\phi_{u,m}(\mathbf{s}_{n+\ell}) = \prod_{i=1}^{|u|} \text{wal}(k_{j_i}^{(m)}, s_{n+\ell}^{(j_i)}),$$

where $2^{m-1} \leq k_{j_1}^{(m)}, \dots, k_{j_{|u|}}^{(m)} < 2^m$. Without loss of generality, we assume that the number of j_i , $1 \leq i \leq |u|$, with $\text{wal}(k_{j_i}^{(m)}, s_{n+\ell}^{(j_i)}) = -1$ is odd. Then, from Lemma 2, the number of j_i , $1 \leq i \leq |u|$, with $\text{wal}(k_{j_i}^{(m)}, s_{n+\ell+2^{m-1}}^{(j_i)}) = -1$ is even because $|u|$ is odd. Thus, the proof is complete. $\square$

Note that $I(\phi_{u,m}) = 0$ for any $u \neq \emptyset$ and $m \geq 1$. From Lemma 3, it follows that the integration error e_N of $\phi_{u,m}$ with $|u|$ odd for any sequence $\mathbf{s}_n$, $n = 0, 1, \dots$, in $\mathfrak{S}_d$ is given by

$$e_N(\mathbf{s}_n, \phi_{u,m}) = \left| \frac{1}{N} \sum_{n=0}^{N-1} \phi_{u,m}(\mathbf{s}_n) \right| = \left| \frac{1}{N} \sum_{n=N-N_m}^{N-1} \phi_{u,m}(\mathbf{s}_n) \right| \leq \frac{\min(2^{m-1}, N)}{N},$$

where N_m is the residue of N modulo 2^m .

We are now ready to prove Theorem 4:

$$\begin{aligned} e_N(\mathbf{s}_n, f) &= \left| \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{s}_n) - I(f) \right| = \left| \frac{1}{N} \sum_{n=0}^{N-1} (f(\mathbf{s}_n) - c_0) \right| \\ &= \left| \frac{1}{N} \sum_{n=0}^{N-1} \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} c_{u,m} \phi_{u,m}(\mathbf{s}_n) \right| \leq \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} \left| \frac{c_{u,m}}{N} \sum_{n=0}^{N-1} \phi_{u,m}(\mathbf{s}_n) \right| \\ &\leq \frac{1}{N} \sum_{\substack{1 \leq |u| \leq d \\ |u| \text{ is odd}}} \sum_{m=1}^{\infty} |c_{u,m}| \min(2^{m-1}, N). \end{aligned}$$

Thus, the proof is complete. $\square$

We should note that a sequence $\mathbf{s}_n$, $n = 1, 2, \dots$, in $\mathfrak{S}_d$ is distributed in the sub-domain $[1/2^m, 1/2^{m-1}]^d$ when n is a multiple of 2^{m-1} but not of 2^m for some $m \geq 1$. Therefore, high-discrepancy sequences employed in the above are *essentially non-uniform* because they are distributed in only a part of the diagonal domain $[0, 1/2]^d \cup [1/2, 1]^d$.

3. Discussion

For a function $f(x_1, \dots, x_d)$ which satisfies

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

there are three approaches to its numerical integration when the dimension d is large.

- *Monte Carlo methods.* We have two types of Monte Carlo methods: uniform random sampling over the whole domain $[0, 1]^d$ or over two sub-domains, $[0, \frac{1}{2}]^d$ and $[\frac{1}{2}, 1]^d$. For both cases, the convergence rate is $O(N^{-1/2})$.
- *Quasi-Monte Carlo or low-discrepancy methods.* This approach provides the convergence rate $O((\log N)^d/N)$ for functions of bounded variation [1, 4–7, 10].
- *High-discrepancy methods.* There are two types of high-discrepancy methods: The first type is to apply low-discrepancy sequences to each of the two sub-domains, $[0, \frac{1}{2}]^d$ and $[\frac{1}{2}, 1]^d$, as the whole domain. The class of (∞, d) -sequences introduced in Proposition 2 can be used for such a purpose. In this case, we get the convergence rate $O((\log N)^d/N)$ for functions of bounded variation. Note that this type is closely related to Hlawka–Mück approach [2]. The second type uses essentially non-uniform sequences such as the class $\mathfrak{S}_d$. For the particular case of $\mathfrak{F}_d$, we have shown the $O(N^{-1})$ convergence rate, which is better than Monte Carlo and quasi-Monte Carlo methods. However, at least at present, nothing is known for functions besides $\mathfrak{F}_d$.

An important consequence from our 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 to satisfy equation (1), there is a possibility to develop faster algorithms based on the ‘high-discrepancy’ approach than Monte Carlo and/or quasi-Monte Carlo (low-discrepancy) methods. There are several applications in practice involving a class of functions in high dimensions which are localized in a

very limited domain. Commonly, we have used the so-called importance sampling techniques including Markov chain Monte Carlo methods for these applications. Unfortunately, all Monte Carlo techniques suffer from the slow convergence rate $O(N^{-1/2})$, while our high-discrepancy approach, which is deterministic, has a potential of the convergence rate $O(N^{-1})$. Therefore, we can consider the high-discrepancy approach as a possible alternative. However, there are many topics to be explored in this new area.

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