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Tezuka, Shu
Faculty of Mathematics, Kyushu University

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S. Tezuka

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Faculty of Mathematics
Kyushu University
Fukuoka, JAPAN

On High-Discrepancy Sequences

Shu Tezuka

Faculty of Mathematics, Kyushu University

6-10-1 Hakozaki, Higashi-ku, Fukuoka-shi, Fukuoka-ken, Japan 812-8581

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.

Key words: discrepancy, high dimensional integrals, Monte Carlo and quasi-Monte Carlo methods, (t, d) -sequences, uniform distribution, Walsh functions

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 suf-

Email address: `tezuka@math.kyushu-u.ac.jp` (Shu Tezuka).

sufficient condition for every function in the class to satisfy the equation (1). From the Information-Based Complexity (IBC) viewpoint, Woźniakowski [9,10] analyzed the average case complexity with respect to the Wiener sheet measure for the integration of this class of functions. The well-known 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 the 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 the 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 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 star discrepancy $D_N^{(d)}$ of the first N points is given by*

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

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

Notice that if the righthand side in the 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 1 *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. Since the sequence is an (∞, d) -sequence which is distributed in only two sub-domains, $[0, \frac{1}{2}]^d$ and $[\frac{1}{2}, 1]^d$, the proof follows.

Note that there are two types of (∞, d) -sequences, i.e., uniform or non-uniform. The sequence introduced in Proposition 1 is a non-uniform (∞, d) -sequence.

We give the following theorems, which motivate 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

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

PROOF. Since

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

for any $k \geq 1$, we have

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

And 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

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

and

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

Thus, the proof is complete. \square

Theorem 2 Suppose that the dimension d is odd. If an L_2 function in d dimensions is written as

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

then we have

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

PROOF. Since

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

for any $k \geq 1$, we have

$$\int_{[0,1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = c_0.$$

And since

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

for any even $k \geq 2$, and

$$\int_0^{1/2} \sin(2\pi kx) dx = - \int_{1/2}^1 \sin(2\pi kx) dx = \frac{1}{k\pi}$$

for any odd $k \geq 1$, we have

$$\int_{[0, \frac{1}{2}]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{c_0}{2^d} + \sum_{\substack{k_1, \dots, k_d \geq 1 \\ \text{all } k_1, \dots, k_d \text{ are odd}}} \frac{c_{k_1, \dots, k_d}}{k_1 \cdots k_d \pi^d},$$

and

$$\int_{[\frac{1}{2}, 1]^d} f(x_1, \dots, x_d) dx_1 \dots dx_d = \frac{c_0}{2^d} + (-1)^d \sum_{\substack{k_1, \dots, k_d \geq 1 \\ \text{all } k_1, \dots, k_d \text{ are odd}}} \frac{c_{k_1, \dots, k_d}}{k_1 \cdots k_d \pi^d}.$$

Since d is odd, the proof is complete. \square

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.

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.

Theorem 3 *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

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

where

$$E_d = \sum_{\substack{0 \leq k_1, \dots, k_d \leq 1 \\ (k_1, \dots, k_d) \neq (0, \dots, 0) \\ k_1 + \dots + k_d \equiv 0 \pmod{2}}} c_{k_1, \dots, k_d}. \quad (3)$$

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

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

and

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

Thus, the proof is complete. \square

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

Definition 2 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 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 4 For any function $f(x_1, \dots, x_d)$ in \mathfrak{F}_d , we have

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

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

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 is a special subset of the class of non-uniform (∞, d) -sequences introduced in Proposition 1. We prove the following theorem.

Theorem 5 *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 generalization 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 $m \geq 1$. For all $n = h 2^m, h = 0, 1, \dots$, 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 the others are identical. Since the generator matrix is nonsingular and lower-triangular, this completes the proof. \square

Lemma 2 *Suppose $m \geq 1$. For all $n = h 2^m, h = 0, 1, \dots$, 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 nonsingular 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

Lemma 3 Suppose $m \geq 1$. Let u be any nonempty 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 5.

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

Thus, the proof is complete.

We should notice that a sequence $\mathbf{s}_n, n = 1, 2, \dots$, in \mathfrak{S}_d is distributed in the sub-domain $[\frac{1}{2^m}, \frac{1}{2^{m-1}}]^d$ 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 $[0, \frac{1}{2}]^d \cup [\frac{1}{2}, 1]^d$.

3 Discussion

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

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

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].
- 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 1 can be used for such 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 the 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 (MCMC) 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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