博士論文（要約）

論文題目
Research on Walsh figure of merit for higher order convergent Quasi-Monte Carlo integration
（高次収束準モンテカルロ積分のための Walsh figure of merit の研究）

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QMC integration is one of the methods for numerical integration (see [5, 12, 15] for example). We approximate the integration value $I(f) = \int_{[0,1)^s} f(x)\,dx$ of a function f by the average

$$I_P(f) = \frac{1}{|P|}\sum_{x\in P} f(x)$$

over a finite point set P. Using QMC integration, we can calculate integration values efficiently in a high dimension s.

In the case $s = 1$, we have many efficient methods for numerical integration. However we can not obtain efficient methods in the case $s > 1$ by applying the methods of the case $s = 1$. In fact, we consider the multidimensional rectangle rule $T_P^s(f) = \frac{1}{n^s}\sum_{1\leq j\leq s, 0\leq t_j\leq n-1} f((\frac{t_j}{n})_{j=1}^s)$, which is the average over the point set $P = \{(\frac{t_j}{n})_{j=1}^s\}_{1\leq j\leq s, 0\leq t_j\leq n-1}$ with its cardinality $N = n^s$. In this case, the integration error $|I(f) - T_P^s(f)|$ is of order $O(N^{-\frac{1}{s}})$ for N. For large s the convergence $N^{-\frac{1}{s}}$ to 0 is very slow as $N \to \infty$. This phenomenon is called the curse of dimensionality (see [5, Chapter 1]).

One method to avoid curse of dimensionality is Monte Carlo (MC) method. We approximate $I(f)$ by the average $I_P(f)$ over a point set P chosen uniformly randomly with its cardinality N. The average of integration error $|I(f)-I_P(f)|$ is of order $O(N^{-\frac{1}{2}})$ for a square integrable function f. But this method gives us the probabilistic error bound. Further the convergence rate $O(N^{-\frac{1}{2}})$ is still slow for some applications and does not reflects regularities of integrands f (see [9, 12] for more information about MC).

Quasi-Monte Carlo (QMC) integration is a deterministic method, which approximate $I(f)$ using a deterministically chosen point set P. QMC gives us a fast convergence rate of integration error reflecting regularities of integrands. In the classical theory, the order of the integration error is known to be $O(N^{-1}\log^{s-1} N)$ for functions f whose partial derivatives are continuous (see [5, 12]). This order is faster than that of MC. Further, when we consider QMC for smoother functions, we can obtain the higher order convergence compared with $O(N^{-1}\log^{s-1} N)$. We study about QMC for smooth functions in this thesis.

1 The main idea to analyze QMC integration error

We consider the QMC integration error

$$\mathrm{Err}(f; P) := I_P(f) - I(f)$$

over a finite point set P in $[0, 1)^s$ for an integrable function $f\colon [0, 1)^s \to \mathbb{R}$. Our main goal is to find a point set P satisfying $|\mathrm{Err}(f; P)|$ is small for a set of functions f. We often assume that a set of functions is a function space, which we denote by H here. We consider the worst case error of H by a point set P

$$wce(H;P) := \sup_{f\in H, \|f\|_H \le 1} |\mathrm{Err}(f;P)|,$$

where $\|f\|_H$ is the norm of H. Then we have the following inequality:

$$|\mathrm{Err}(f;P)| \le wce(H;P)\|f\|_H.$$

If we can find a point set $P = P_0$ with $wce(H;P)$ small, we can expect that $|\mathrm{Err}(f;P_0)|$ is small for any $f \in H$.

Since it is difficult to analyze the structure of $wce(H;P)$, we often treat an upper bound $w(H;P)$ on $wce(H;P)$. Using $w(H;P)$, we obtain the following form of inequalities

$$|\mathrm{Err}(f;P)| \le w(H;P)\|f\|_H. \tag{1}$$

We call an inequality (1) a Koksma-Hlawka type inequality (see [5, 8]).

In QMC analysis, we often use a special class of point sets. In particular we assume that point sets are digital nets [12] in this thesis. A digital net is a point set which is identified with $\mathbb{Z}_b$-module $(\mathbb{Z}_b)^m$. We write $\mathbb{Z}_b = \mathbb{Z}/\mathbb{Z}_b$.

Definition 1.1 (digital net over $\mathbb{Z}_b$)**.** *Let $n, m \ge 1, b \ge 2$ be integers with $n \ge m$. Let $0 \le h < b^m$ be an integer and $C_1, \dots, C_s$ be $n \times m$ matrices over the finite group $\mathbb{Z}_b$. We write the b-adic expansion $h = \sum_{j=1}^m h_j b^{j-1}$ and take a vector $\mathbf{h} = (h_1, \dots, h_m) \in (\mathbb{Z}_b^m)^\top$, where h_j is considered to be an element in $\mathbb{Z}_b$. For $1 \le i \le s$, we define the vector $(y_{h,i,1}, \dots, y_{h,i,n}) = \mathbf{h} \cdot (C_i)^\top$ and a real number $x_i(h) = \sum_{1\le j\le n} y_{h,i,j} b^{-j} \in [0,1)$, where $y_{h,i,j}$ is considered to be an element of $\{0, \dots, b-1\} \subset \mathbb{Z}$. Then we define a digital net P by $\{x_0, \cdots, x_{b^m-1}\}$ where $\mathbf{x}_h = (x_i(h))_{1\le i\le s}$. We call $\{C_i\}_{i=1}^s$ generating matrices of a digital net P.*

From now on, we use the symbol $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. We define the dual net $P^\perp$ [4, 13] of a digital net P, which is essential to analyze QMC integration error by P:

Definition 1.2 (dual net)**.** *Let $\{C_i\}_{i=1}^s$ be generating matrices of a digital net P. We define a dual net $P^\perp$ as follows;*

$$P^\perp := \{k = (k_1, \dots, k_s) \in \mathbb{N}_0^s \mid C_1^\top \vec{k}_1 + \cdots + C_s^\top \vec{k}_s = \mathbf{0} \in \mathbb{Z}_b^m\},$$

where $\vec{k}_i = (\kappa_{i,1}, \dots, \kappa_{i,n})^\top$ for k_i with b-adic expression $k_i = \sum_{j\ge1} \kappa_{i,j} b^{j-1}$. Here $\kappa_{i,j}$ is considered to be an element of $\mathbb{Z}_b$.

2 Previous results about QMC

In the classical theory, many researchers studied the integration error of a function with continuous partial derivatives up to first order in each variable (they also treat wider function spaces, see [6, 7]). For these functions, the following Koksma-Hlawka type inequality holds;

$$|\mathrm{Err}(f;P)| \le D^*(P)\|f\|_{KH},$$

where the norm $\|f\|_{KH}$ is defined using partial derivatives of f and $D^*(P)$ is called a star-discrepancy. There are also many constructions of P whose $D^*(P)$ is of order $O(N^{-1}\log^{s-1} N)$ in terms of the cardinality N of a point set P (see [5, 12]). This order is known to be best possible up to powers of $\log N$ (see [1]).

Recently, an extension to smooth functions was shown in [2, 3, 5]. Consider functions f whose mixed partial derivatives up to order α in each variable are continuous, which we call an α-smooth function here (they also treat wider function spaces in [2, 3, 5]). For these functions f and a digital net P over $\mathbb{Z}_b$, the following Koksma-Hlawka inequality holds;

$$|\mathrm{Err}(f;P)| \le C_{s,b,\alpha} W_\alpha(P)\|f\|_\alpha, \tag{2}$$

where $C_{s,b,\alpha}$ is a constant depending on b, s, α and the norm $\|f\|_\alpha^2$ is defined as $\sum_{i=0}^{\alpha}\left|\int_0^1 f^{(i)}(x)\,dx\right|^2 + \int_0^1 \left|f^{(i)}(x)\right|^2 dx$ for $s = 1$ (see [3] for the complete form of the norm). Here $W_\alpha(P)$ is defined as follows;

$$W_\alpha(P) := \sum_{k\in P^\perp\setminus\{0\}} b^{-\mu_\alpha(k)},$$

where $\mu_\alpha(k)$ is the weight function of $k = (k_i)_{i=1}^s \in \mathbb{N}_0^s$;

$$\mu_\alpha(k) = \sum_{i=1}^{s}(a_{i,1} + \cdots + a_{i,\min(\alpha,N_i)})$$

for b-adic expansion $k_i = \sum_{j=1}^{N_i} \kappa_{i,j} b^{a_{i,j}}, (\kappa_{i,j} \neq 0, a_{i,1} > \cdots > a_{i,N_i})$.

The construction method of digital nets whose $W_\alpha(P) \in O(N^{-\alpha}\log^{\alpha s} N)$ in terms of the cardinality N of a point set P is known. (see [2, 3]). This order $O(N^{-\alpha}\log^{\alpha s} N)$ is also known to be best possible up to powers of $\log N$ (see [14]). See also [3] for more background on higher order QMC rules.

It is important to obtain an optimal order of integration error, and point sets which attain its order. But we can not take the cardinality N large enough in some applications. Thus we also have to find good point sets P for small N. Walsh figure of merit (WAFOM) is introduced for that purpose.
WAFOM is defined for a digital net over $\mathbb{Z}_2$ [10], then Suzuki generalized WAFOM for a digital net over $\mathbb{Z}_b$ in [16]. Let P be a digital net over $\mathbb{Z}_b$. WAFOM(P) is defined as the approximation of $W_n(P)$ for large n;

$$\mathrm{WAFOM}(P) := \sum_{k=(k_i)_{i=1}^s\in P^\perp\setminus\{0\}, k_i<b^n} b^{-\mu_\infty(k)} = \sum_{k=(k_i)_{i=1}^s\in P^\perp\setminus\{0\}, k_i<b^n} b^{-\mu_n(k)}.$$

Here we define that $\mu_\infty(k)$ is the weight function of $k = (k_i)_{i=1}^s \in \mathbb{N}_0^s$;

$$\mu_\infty(k) = \sum_{i=1}^{s}(a_{i,1} + \cdots + a_{i,N_i}),$$

which can be seen as the limitation of $\mu_\alpha(k)$. Notice that $\mu_\infty(k) = \mu_n(k)$ for k with $k_i < b^n$.
WAFOM depends on n, which is the parameter of a digital net P and also the smoothness of a function f. For n-smooth functions f, the following 'discretized' Koksma-Hlawka inequality holds:

$$|\mathrm{Err}(f_n; P)| \leq \mathrm{WAFOM}(P)\|f\|_n.$$

Here f_n is the discretized function of f, which satisfies that $|f - f_n| \in O(b^{-n})$ if f is Lipschitz continuous (see [10, 16] for the definition of f_n). When we take n large enough, $|\mathrm{Err}(f_n; P) - \mathrm{Err}(f; P)|$ can be ignored for n-smooth functions f. Thus WAFOM(P) is an approximate bound on $|\mathrm{Err}(f; P)|$ for n-smooth functions f.
The merit of WAFOM is the computable formula [10, 16]. It enables us to calculate WAFOM in $O(ns|P|)$ arithmetic operations. Thus we can find a digital net P with small WAFOM(P) by computer search.

3 Main results of this thesis

In this thesis we unveiled the important properties of WAFOM(P) for a digital net P over $\mathbb{Z}_2$. And we make the new Koksma-Hlawka inequality for α smooth functions.

【 Main Result 1 】 : Existence of Higher Order Convergent Quasi-Monte Carlo Rules via Walsh Figure of Merit

The content including the following content has already appeared in [11]. We show the existence of digital nets over $\mathbb{Z}_2$ with small WAFOM values.

Theorem 3.1. *There are explicit constants E, C, D such that for any $m \geq 9s$, there is digital nets P of size $N = 2^m$ with*

$$\mathrm{WAFOM}(P) \leq E \cdot 2^{-Cm^2/s + Dm} = E \cdot N^{-C(\log_2 N)/s + D}.$$

The proof of this theorem is based on the idea that WAFOM(P) is bounded by the minimum weight $\delta_{P^\perp}$ of a digital net P;

$$\mathrm{WAFOM}(P) \leq C_3 \cdot 2^{-C_1\delta_{P^\perp} + C_2\sqrt{s\delta_{P^\perp}}},$$

where $\delta_{P^\perp}$ is defined as

$$\delta_{P^\perp} := \min_{k=(k_i)\in P^\perp \setminus \{0\}, k_i < 2^\infty} \mu_n(k).$$

Then we prove the existence of digital nets P with large minimum weight $\delta_{P^\perp} \geq C_4 m^2/s$ by a probabilistic argument. Combining these, we obtain the result.

【 Main Result 2 】 : A lower bound on WAFOM

The content including the following result has already appeared in [17]. We show a lower bound on WAFOM for digital nets P over $\mathbb{Z}_2$;

Theorem 3.2. *Let C' be an arbitrary real number greater than $1/2$. If $m/s \geq (\sqrt{C'+1/16}+3/4)/(C'-1/2)$, then for any digital net P over $\mathbb{Z}_2$ with its size $N = 2^m$, we have*

$$\mathrm{WAFOM}(P) \geq 2^{-C'm^2/s} = N^{-C'\log N/s}.$$

Combing the above theorem, we can see that $O(N^{-A\log N/s})$ is the optimal order of WAFOM in terms of the size N, up to a constant A. This order beyonds the order $O(N^{-\alpha}\log^{s\alpha} N)$ of integration errors for α-smooth functions with fixed α. Since WAFOM(P) approximately bounds on $\mathrm{Err}(f;P)$ for large enough n, this result implies that there is a smooth function space whose functions f satisfy $\mathrm{Err}(f;P) \in O(N^{-A\log N/s})$. This order also gives us the criteria for determining whether digital nets are good for QMC or not.

This theorem is also proved by using the minimum weight $\delta_{P^\perp}$ for a digital net P over $\mathbb{Z}_2$. By the definition of WAFOM, we have that

$$\mathrm{WAFOM}(P) \geq 2^{-\delta_{P^\perp}}.$$

Thus an upper bound on $\delta_{P^\perp}$ gives a lower bound on WAFOM. To obtain an upper bound on $\delta_{P^\perp}$, we need a subset $W \subset \{k = (k_i) \in P^\perp \backslash \{0\} \mid k_i < 2^n\}$ such that $P^\perp \cap W \neq \{O\}$ for any digital net P with its cardinality $N = 2^m$. If we can find such a subset W, we obtain $\delta_{P^\perp} \leq \max_{X\in W} \mu_\infty(X)$. The proof is finished by making the subset $W = W_0$ satisfying $\max_{X\in W_0} \mu_\infty(X) = C'm^2/s$.

【 Main Result 3 】 : An Efficient Approximation of Walsh Figure of Merit with Derivation-sensitivity Parameter

We show that WAFOM can be computed by the integration error of an exponential function;

Theorem 3.3. *There are explicit constants U, L such that*

$$L^s \leq \frac{\mathrm{Err}(\exp(-2\sum_{i=1}^s x_i); P)}{\mathrm{WAFOM}_\infty(P)} \leq U^s,$$

where $\mathrm{WAFOM}_\infty(P) = \sum_{k=(k_i)\in P^\perp\backslash\{0\}} 2^{-\mu_\infty(k)}$ *for any digital net P over $\mathbb{Z}_2$, and the values of L and U are approximately* 0.388 *and* 0.432.

Since it holds that $|\mathrm{WAFOM}_\infty(P) - \mathrm{WAFOM}(P)| \in O(2^{-n})$, WAFOM$(P)$ is approximated by $\mathrm{Err}(\exp(-2\sum_{i=1}^s x_i); P)$ for large n. Thus we have only to compute $\mathrm{Err}(\exp(-2\sum_{i=1}^s x_i); P)$ instead of WAFOM(P) in order to find low WAFOM point sets.

We also show that WAFOM is the worst case error for some smooth function space by using this result. Further we treat the generalized versions of WAFOM with 'derivation-sensitivity parameters'.

The proof of this theorem is based on Walsh coefficients $\hat{f}(k)$, which is one of the generalized Fourier coefficients (see Definition 3.4). The integration error for a smooth function f by a digital net P can be written by Walsh coefficients $\hat{f}(k)$; $\mathrm{Err}(f;P) = \sum_{k \in P^\perp \setminus \{0\}} \hat{f}(k)$. In general it is difficult to calculate the explicit value $\hat{f}(k)$ for f. But for an exponential function $g_a = \exp(a \sum_{i=1}^s x_i)$, $\hat{g_a}(k)$ can be calculated and we obtain the following estimate for $g_2 = \exp(-2 \sum_{i=1}^s x_i)$;

$$L^s \leq \frac{\hat{g_2}(k)}{2^{-\mu_\infty(k)}} \leq U^s.$$

Combing these, we get the theorem.

【 Main Result 4 】 : Bounds on Walsh coefficients by dyadic difference and a new Koksma-Hlawka type inequality for Quasi-Monte Carlo integration

The article including the following content is submitted (see [18]). We analyze the integration error for an α-smooth function by a digital net and make a new Koksma-Hlawka inequality.

In order to analyze the integration error for an α-smooth function by a digital net, we need the important tools:

Definition 3.4 (Walsh functions and Walsh coefficients)**.** *Let $f\colon [0,1)^s \to \mathbb{R}$ and $k = (k_1, \dots, k_s) \in \mathbb{N}_0^s$. We define the k-th Walsh function* wal_k *by*

$$\mathrm{wal}_k(x) := \prod_{i=1}^s \Big(\exp(\frac{2\pi i}{b}) \Big)^{\sum_{j\geq 1} \beta_{i,j} \kappa_{i,j}},$$

where for $1 \leq i \leq s$, we write the b-adic expansion of k_i by $k_i = \sum_{j \geq 1} \kappa_{i,j} b^{j-1}$ and x_i by $x_i = \sum_{j \geq 1} \beta_{i,j} b^{-j}$, where for each i, infinitely many of the digits $\beta_{i,j}$ are different from $b-1$. By using Walsh functions, we define the k-th Walsh coefficient $\hat{f}(k)$;

$$\hat{f}(k) := \int_{[0,1)^s} f(x) \cdot \overline{\mathrm{wal}_k(x)}\, dx,$$

where $\overline{\mathrm{wal}_k(x)}$ denotes the complex conjugate of $\mathrm{wal}_k(x)$*.*

We see that the integration error $\mathrm{Err}(f;P)$ by a digital net P can be represented by Walsh coefficients $\hat{f}(k)$ as follows ([5, Chapter 15]);

$$\mathrm{Err}(f;P) = \sum_{k \in P^\perp \setminus \{0\}} \hat{f}(k).$$

Here we assume that we get an inequality of the form $|\hat{f}(k)| \leq w(k)\|f\|$, where $\|f\|$ is a norm of f and $w(k)$ is a weight function of k. Then we have a Koksma-Hlawka type inequality as

$$|\mathrm{Err}(f;P)| \leq w(H_\alpha;P)\|f\|,$$

where

$$w(H_\alpha;P) = \sum_{k \in P^\perp \setminus \{0\}} w(k).$$

For an α-smooth functions f, it is well known bounds [2, 5] on $\hat{f}(k)$;

$$|\hat{f}(k)| \leq C_{b,s,\alpha} b^{-\mu_\alpha(k)} \|f\|_\alpha, \tag{3}$$

where $C_{b,s,\alpha}, \|f\|_\alpha, \mu_\alpha(k)$ are already seen in (2). Combining this inequality and the above computation, we have the Koksma-Hlwaka inequality (2).

We improve the inequality (2) for a digital net over $\mathbb{Z}_2$: For $k = (k_i)_{i=1}^s \in \mathbb{N}_0^s$ with its dyadic expansion $k_i = \sum_{j=1}^{N_i} 2^{a_{i,j}}$, we have

$$|\hat{f}(k)| \leq 2^{\frac{s}{p}} \cdot 2^{-\mu_\alpha(k) - \sum_{i=1}^s \min(\alpha, N_i)} \cdot \|f^{(\min(\alpha,N_1),\ldots,\min(\alpha,N_s))}\|_{L^p}, \tag{4}$$

where $1 \leq p \leq \infty$ and $\|\cdot\|_{L^p}$ is the L^p norm. This bound (4) is better than (3) under some condition. Using this bound, we have the following Koksma-Hlawka inequality;

Theorem 3.5. *For $\alpha \geq 2$, a digital net P over $\mathbb{Z}_2$ and an α-smooth function f, we have*

$$|\mathrm{Err}(f;P)| \leq 2^{\frac{s}{p}} \cdot W'_\alpha(P) \cdot \sup_{n_i \leq \alpha} \|f^{(n_1,\cdots,n_s)}\|_{L^p},$$

where $W'_\alpha(P) = \sum_{k \in P^\perp \setminus \{0\}} 2^{-\mu_\alpha(k) - \sum_{i=1}^s \min(\alpha, N_i)}$.

This is the improved Koksma-Hlawka inequality obtained by the improved bounds on Walsh coefficients. In fact, this inequality holds for $\alpha = \infty$, though (2) is not proven in the case $\alpha = \infty$. Further, it happens that $\|f\|_\alpha$ is much larger than $\sup_{(n_i)_{i=1}^s, n_i \leq \alpha} \|f^{(n_1,\ldots,n_s)}\|_{L^p}$ since $\|f\|_\alpha$ is the summation of sn positive terms for large α . For example, when $f = \exp(-x)$, $\sup_{n_i \leq \alpha} \|f^{(n_1,\ldots,n_s)}\|_{L^p} = (1-e^{-p})/p)^{1/p}$ while $\|f\|_\alpha = ((\alpha+1)(1-e^{-1})^2 + (1-e^{-2})/2)^{1/2}$. In this case, if we take α large enough, $\sup_{n_i \leq \alpha} \|f^{(n_1,\ldots,n_s)}\|_{L^p} / \|f\|_n$ goes to 0.

The inequality (4) follows from the formula for the Walsh coefficients by dyadic differences. Dyadic difference is defined as follows;

Definition 3.6 (dyadic difference)**.** *Let $s, n, i \in \mathbb{N}$ with $i \leq s$. For a function $g\colon [0,1)^s \to \mathbb{R}$, we define the dyadic difference $\partial_{i,n}(g)$ by*

$$\partial_{i,n}(g)(x_1,\ldots,x_s) := \frac{g(x_1,\ldots,x_i \oplus 2^{-n},\ldots,x_s) - g(x_1,\ldots,x_i,\ldots,x_s)}{2^{-n}}.$$

Here we write $z \oplus 2^{-n} := z + 2^{-n}(-1)^{z_n}$ for z having dyadic expansion $z = \sum_{j=1}^\infty z_j 2^{-j}$, where infinitely many digits z_j are 0.

By dyadic differences, we can obtain the formula

$$\widehat{\partial_{i,a_{i,j}+1}f}(k) = 2^{-a_{i,j}-2}\hat{f}(k),$$

where $k = (k_i)_{i=1}^s, k_i = \sum_{j=1}^{N_i} 2^{a_{i,j}}, a_{i,1} > \cdots > a_{i,N_i}$. This is analogous to the formula between Fourier coefficients and derivatives. The inequality (4) is derived by replacing dyadic differences with derivatives.

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