Quasi-Monte Carlo point sets with small $t$-values and WAFOM

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Abstract

The $t$-value of a $(t,m,s)$-net is an important criterion of point sets for quasi-Monte Carlo integration, and many point sets are constructed in terms of $t$-values, as this leads to small integration error bounds. Recently, Matsumoto, Saito, and Matoba proposed the Walsh figure of merit (WAFOM) as a quickly computable criterion of point sets that ensure higher order convergence for function classes of very high smoothness. In this paper, we consider a search algorithm for point sets whose $t$-value and WAFOM are both small so as to be effective for a wider range of function classes. For this, we fix digital $(t,m,s)$-nets with small $t$-values (e.g., Sobol’ or Niederreiter–Xing nets) in advance, apply random linear scrambling, and select scrambled digital $(t,m,s)$-nets in terms of WAFOM. Experiments show that the obtained point sets improve the rates of convergence for smooth functions and are robust for non-smooth functions.

Keywords: Quasi-Monte Carlo method, Multivariate numerical integration, Digital net, $(t,m,s)$-net, Walsh figure of merit

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1. Introduction

For a Riemann integrable function \( f : [0, 1)^s \to \mathbb{R} \), we consider the integral \( \int_{[0,1)^s} f(x)dx \) and its approximation by quasi-Monte Carlo integration:

\[
\int_{[0,1)^s} f(x)dx \approx \frac{1}{N} \sum_{k=0}^{N-1} f(x_k),
\]

where the point set \( P := \{x_0, \ldots, x_{N-1}\} \subset [0,1)^s \) is chosen deterministically.

A typical quasi-Monte Carlo point set \( P \) is a low-discrepancy point set based on the \( t \)-value of a \((t, m, s)\)-net. Thus, the \( t \)-value is probably the most important criterion of quasi-Monte Carlo point sets \([4, 6, 17]\). Matsumoto, Saito, and Matoba \([14]\) recently proposed the Walsh figure of merit (WAFOM) as another criterion of quasi-Monte Carlo point sets ensuring higher order convergence for function classes of very high smoothness. WAFOM is also quickly computable, and this efficiency enables us to search for quasi-Monte Carlo point sets using a random search. As an analogy to coding theory, since a random search is easier than a mathematical construction (e.g., the success of low-density parity-check codes), Matsumoto et al. also searched for point sets at random by minimizing WAFOM. In the same spirit, Harase and Ohori \([11]\) searched for low-WAFOM point sets with extensibility (i.e., the number of points may be increased while the existing points are retained). In numerical experiments, these point sets are significantly effective for low-dimensional smooth functions. In fact, as shown later (in Remark \([2]\), low-WAFOM point sets based on a simple random search do not always have small \( t \)-values in the framework of \((t, m, s)\)-nets, and such point sets are sometimes inferior to classical \((t, m, s)\)-nets for non-smooth functions.

In this paper, we search for point sets whose \( t \)-value and WAFOM are both small, so as to be effective for a wider range of function classes, i.e., point sets combining the advantages of good \((t, m, s)\)-nets and low-WAFOM point sets. For this, we fix suitable digital \((t, m, s)\)-nets (e.g., Sobol’ or Niederreiter–Xing nets) in advance and apply random linear scrambling with non-singular lower triangular matrices that preserves \( t \)-values. Our key approach is to select good point sets from the scrambled digital \((t, m, s)\)-nets in terms of WAFOM. Our numerical experiments show that the obtained point sets improve the rates of convergence for smooth functions and are robust for non-smooth functions.
The rest of this paper is organized as follows. In Section 2, we briefly recall the definitions of digital \((t, m, s)\)-nets and WAFOM. Section 3 is devoted to our main result: a search for low-WAFOM point sets with small \(t\)-values using linear scrambling. In Section 4, we compare between our new point sets and other quasi-Monte Carlo point sets by using the Genz test function package \([7, 8]\). Section 5 concludes the paper with some directions for future research.

2. Notations

2.1. Digital \((t, m, s)\)-nets

For use in later sections, we briefly recall the definitions of digital \((t, m, s)\)-nets. Let \(s\) and \(n\) be positive integers. Let \(\mathbb{F}_2 := \{0, 1\}\) be the two-element field, and \(V := \mathbb{F}_2^{s \times n}\) the set of \(s \times n\) matrices. Let us denote \(x \in V\) by \(x := (x_{i,j})_{1 \leq i \leq s, 1 \leq j \leq n}\) with \(x_{i,j} \in \mathbb{F}_2\). We identify \(x \in V\) with the \(s\)-dimensional point
\[
\left(\sum_{j=1}^{n} x_{1,j} 2^{-j} + 2^{-n-1}, \ldots, \sum_{j=1}^{n} x_{s,j} 2^{-j} + 2^{-n-1}\right) \in [0, 1)^s.
\]
Note that \(n\) corresponds to the precision. Note also that the points are shifted by \(2^{-n-1}\) because we will later consider WAFOM (see \([14, \text{Remark 2.2}]\)). To construct \(P := \{x_0, x_1, \ldots, x_{2^m-1}\} \subset [0, 1)^s\), we often use the following construction scheme called the \textit{digital net}.

**Definition 1 (Digital net).** Consider \(n \times m\) matrices \(C_1, \ldots, C_s \in \mathbb{F}_2^{n \times m}\). For \(k = 0, 1, \ldots, 2^m - 1\), let \(k = \sum_{l=0}^{m-1} k_l 2^l\) with \(k_l \in \mathbb{F}_2\) be the expansion of \(k\) in base 2. We set \(k := \{k_0, \ldots, k_{m-1}\} \in \mathbb{F}_2^m\), where \(\cdot^t\) represents the transpose. We set \(x_k := \{C_1 k, \ldots, C_s k\} \in V\). Then, the point set \(P := \{x_0, \ldots, x_{2^m-1}\}\) is called a \textit{digital net} over \(\mathbb{F}_2\) and \(C_1, \ldots, C_s\) are the \textit{generating matrices} of the digital net \(P\).

Throughout this paper, we assume \(P\) is a digital net. Note that \(P \subset V\) is an \(\mathbb{F}_2\)-linear subspace of \(V\).

**Definition 2 \((t, m, s)\text{-net}\).** Let \(s \geq 1\), and \(0 \leq t \leq m\) be integers. Then, a point set \(P\) consisting of \(2^m\) points in \([0, 1)^s\) is called a \((t, m, s)\text{-net}\) (in base 2) if every subinterval \(J = \prod_{j=1}^{s} [a_j 2^{-d_j}, (a_j + 1)2^{-d_j})\) in \([0, 1)^s\) with integers \(d_j \geq 0\) and \(0 \leq a_j < 2^{d_j}\) for \(1 \leq j \leq s\) and of volume \(2^{t-m}\) contains exactly
2^t points of \( P \). If \( t \) is the smallest value such that \( P \) is a \((t, m, s)\)-net, then we call this the \( t \)-value (or exact quality parameter). If \( P \) is a digital net, it is called a digital \((t, m, s)\)-net.

As a criterion, \( P \) is well distributed if the \( t \)-value is small. In this framework, from the Koksma–Hlawka inequality and estimation of star-discrepancies, the upper bound on the absolute error of (1) is \( O(2^t(\log N)^{s-1}/N) \) (see [6, 17] for details). There are many studies on generating matrices of digital \((t, m, s)\)-nets, e.g., Sobol’ nets [24], Niederreiter nets [17], and Niederreiter–Xing nets [26]. There are also some algorithms for computing \( t \)-values of digital nets [3, 22].

2.2. WAFOM

Matsumoto et al. [14] proposed WAFOM as a computable criterion of quasi-Monte Carlo point sets constructed by digital nets \( P \). WAFOM has the potential ability to ensure higher order convergence than \( O(N^{-1}) \) for function classes of very high smoothness (so-called \( n \)-smooth functions). In a recent talk, Yoshiki [28] modified the definition of WAFOM resulting in a more explicit upper bound for integration errors. Thus, throughout this paper, we adopt this new result as our WAFOM value.

**Definition 3 (WAFOM).** Let \( P \subset V \) be a digital net. For \( \mathbf{x} = (x_{i,j}) \in P \), the (modified) WAFOM (or Walsh figure of merit) is defined as

\[
\text{WAFOM}(P) := \frac{1}{|P|} \sum_{\mathbf{x} \in P} \left\{ \prod_{1 \leq i \leq s} \prod_{1 \leq j \leq n} (1 + (-1)^{x_{i,j}}2^{-j-1}) - 1 \right\}.
\]

(2)

This criterion is computable in \( O(nsN) \) arithmetic operations, where \( N := |P| \), and is computable in \( O(sN) \) steps when using look-up tables (see [11]).

Next, we recall the \( n \)-digit discretization \( f_n \) of \( f \) by following [14, Section 2]. For \( \mathbf{x} = (x_{i,j})_{1 \leq i \leq s, 1 \leq j \leq n} \in V \), we define the \( s \)-dimensional subinterval \( I_{\mathbf{x}} \subset [0, 1)^S \) by

\[
I_{\mathbf{x}} := \left[ \sum_{j=1}^{n} x_{1,j}2^{-j}, \sum_{j=1}^{n} x_{1,j}2^{-j} + 2^{-n} \right] \times \cdots \times \left[ \sum_{j=1}^{n} x_{s,j}2^{-j}, \sum_{j=1}^{n} x_{s,j}2^{-j} + 2^{-n} \right].
\]

For a Riemann integrable function \( f : [0, 1)^s \to \mathbb{R} \), we define its \( n \)-digit discretization \( f_n : V \to \mathbb{R} \) by \( f_n(\mathbf{x}) := (1/\text{Vol}(I_{\mathbf{x}})) \int_{I_{\mathbf{x}}} f(\mathbf{x}) \, d\mathbf{x} \). This is the
average value of $f$ over $I_x$. When $f$ is Lipschitz continuous, it can be shown [14] that the discretization error between $f$ and $f_n$ on $I_x$ is negligible if $n$ is sufficiently large (e.g., when $n \geq 30$). Thus, for such $f : [0, 1)^s \to \mathbb{R}$ and large $n$, we may consider (1/|P|) $\sum_{x \in P} f_n(x)$.

Here, we assume that $f$ is an $n$-smooth function (see [2] and [6, Ch. 14.6] for the definition). Yoshiki [28] gave the following Koksma–Hlawka type inequality by improving Dick’s inequality ([3, Section 4.1] and [14, (3.7)]):

$$\left| \int_{[0,1)^s} f(x) dx - \frac{1}{|P|} \sum_{x \in P} f_n(x) \right| \leq \sup_{0 \leq N_1, \ldots, N_s \leq n} ||f^{(N_1, \ldots, N_s)}||_\infty \cdot \text{WAFOM}(P),$$

where $||f||_\infty$ is the infinity norm of $f$ and $f^{(N_1, \ldots, N_s)} := \partial^{N_1} \cdots \partial^{N_s} f / \partial x_1^{N_1} \cdots \partial x_s^{N_s}$.

**Remark 1.** In [14], WAFOM is originally defined by replacing $2^{-j-1}$ in [2] with $2^{-j}$. Following the discussions in [15, 25, 27], the best (i.e., smallest) value of $\log(\text{WAFOM}(P))$ is $O(-m^2/s)$ for $P$ with $|P| = 2^m$. Thus, WAFOM can be used to search a digital net $P$ with higher order convergence than $O(N^{-1})$ for $n$-smooth functions.

### 3. Scrambling methods

In previous works, Matsumoto et al. [14] and Harase and Ohori [11] searched for low-WAFOM point sets using only WAFOM as a criterion. In fact, the point sets obtained in these ways do not always have small $t$-values as $(t, m, s)$-nets. In this section, we take into account the structure of $(t, m, s)$-nets, and search for low-WAFOM point sets with small $t$-values. For this, we consider the following transformation, known as linear scrambling.

**Proposition 1 ([19]).** Let $C_1, \ldots, C_s \in \mathbb{F}_2^{n \times m}$ be generating matrices of a digital $(t, m, s)$-net. Let $L_1, \ldots, L_s \in \mathbb{F}_2^{n \times n}$ be non-singular lower triangular matrices. Then, the digital net with generating matrices $L_1 C_1, \ldots, L_s C_s \in \mathbb{F}_2^{n \times m}$ is also a $(t, m, s)$-net.

Linear scrambling preserves the $t$-values, so we cannot distinguish whether scrambled nets are good using $t$-values itself. Here, WAFOM can be applied to the assessment of linearly scrambled digital $(t, m, s)$-nets. Our algorithm proceeds as follows:

1. Fix a digital $(t, m, s)$-net with a small $t$-value in advance.
2. Generate $L_1, \ldots, L_s$ at random $M$ times, and construct $P$ from $L_1C_1, \ldots, L_sC_s$.
3. Select the point set $P$ with the smallest WAFOM($P$).

In this case, note that the point sets $P$ are not extensible.

As an example, we set $(s, n, M) = (5, 32, 100000)$ and compare the WAFOM values of the following point sets $P$:

- (a) Niederreiter–Xing nets [26] implemented by Pirsic [21].
- (b) Sobol’ nets with better two-dimensional projections [12].
- (c) Naive low-WAFOM point sets based on a random search [11].
- (d) Scrambled Niederreiter-Xing nets given by the above procedure.
- (e) Scrambled Sobol’ nets given by the above procedure.

Figure 1 plots the WAFOM values. This shows that (c)–(e) have similar values. Taking a closer look at the figure, the WAFOM values of the Sobol’ nets (without linear scrambling) are rather large. This is because the generating matrices $C_1, \ldots, C_s \in \mathbb{F}_2^{n\times m}$ of Sobol’ nets are non-singular upper triangular, and hence the lower bits in their output are all zero. Consequently, WAFOM($P$) tends to be large in (2). Roughly speaking, the slope of the Sobol’ nets is $O(N^{-1})$. In fact, the WAFOM values of the Niederreiter–Xing nets are already small, so we obtain higher order convergence rates using non-scrambled Niederreiter–Xing nets. However, by selecting suitable scrambling matrices, further improvements can be obtained for large values of $m$.

**Remark 2.** Low-WAFOM point sets based on a simple random search do not always possess small $t$-values, particularly for larger $s$ and $m$. Table 1 gives a summary of the $t$-values of the above point sets for $s = 5$. As described in [11], the naive low-WAFOM point sets were searched by inductively determining the columns vectors of $C_1, \ldots, C_s$ in terms of WAFOM, thus allowing extensibility. Because we did not consider the structure of the $(t, m, s)$-nets in advance, the $t$-values are rather large. Matsumoto–Saito–Matoba (non-extensible) sequential generators [14] exhibit a similar tendency. Nevertheless, such low-WAFOM point sets are effective for smooth functions (see the next section for details).

**Remark 3.** In two pioneering papers, Dick [1, 2] proposed higher order digital nets and sequences that achieve a convergence rate of $O(N^{-\alpha}(\log N)^{\alpha s})$ for $\alpha$-smooth functions ($\alpha \geq 1$) by considering the decay of the Walsh coefficients. For this, he described an explicit construction for generating
matrices, called *interlacing*. Namely, we prepare \( s \alpha \) generating matrices \( C_1, \ldots, C_{s \alpha} \in \mathbb{F}_2^{m \times m} \) of a digital \((t, m, s \alpha)\)-net in advance. These are converted to the matrices \( C_1^{(\alpha)}, \ldots, C_{s \alpha}^{(\alpha)} \in \mathbb{F}_2^{m \alpha \times m} \) by rearranging the row vectors of \( \alpha \) successive generating matrices. Then, the digital net with \( C_1^{(\alpha)}, \ldots, C_{s \alpha}^{(\alpha)} \) achieves a convergence rate of \( O(N^{-\alpha}(\log N)^{\alpha s}) \). From [6, Proposition 15.8], such a digital net is a classical digital \((t', m, s)\)-net with \( t' \leq t \). However, when \( \alpha \) or \( s \) is large, the exact quality parameter \( t' \) might become large compared with the best possible \( t \)-value in the framework of classical \((t, m, s)\)-nets. The last two rows of Table 1 give the \( t \)-values of interlaced Niederreiter–Xing nets for \( \alpha = 2 \) and 3. Our scrambling approach has the advantages that the exact quality parameters \( t \) do not increase and higher order convergences can be expected.

**Remark 4.** Goda, Ohori, Suzuki, and Yoshiki [10] proposed a variant of WAFOM from the view point of the mean square error for digitally shifted digital nets. They defined the criterion by replacing 2 in [2] with 4. Thus, this is applicable to our approach in a similar manner.
4. Numerical results

To evaluate the point sets (a)–(e) described in Section 3, we applied the Genz test package [7, 8]. This has been used in many studies (e.g., [18, 21, 23, 16]), and was also analyzed from a theoretical perspective in [20]. Thus, we investigate six different test functions defined over \([0, 1)^s\). These are:

- Oscillatory: \(f_1(x) = \cos(2\pi u_1 + \sum_{i=1}^s a_i x_i)\),
- Product Peak: \(f_2(x) = \prod_{i=1}^s \left[1/(a_i^{-2} + (x_i - u_i)^2)\right]\),
- Corner Peak: \(f_3(x) = (1 + \sum_{i=1}^s a_i x_i)^{-1}\),
- Gaussian: \(f_4(x) = \exp(-\sum_{i=1}^s a_i^2 (x_i - u_i)^2)\),
- Continuous: \(f_5(x) = \exp(-\sum_{i=1}^s a_i |x_i - u_i|)\),
- Discontinuous: \(f_6(x) = \begin{cases} 0, & \text{if } x_1 > u_1 \text{ or } x_2 > u_2, \\ \exp(\sum_{i=1}^s a_i x_i), & \text{otherwise}. \end{cases}\)

In these functions, we have two parameters, i.e., the difficulty parameters \(a = (a_1, \ldots, a_s)\) and the shift parameters \(u = (u_1, \ldots, u_s)\). We generate \(a = (a_1, \ldots, a_s)\) and \(u = (u_1, \ldots, u_s)\) as uniform random vectors in \([0, 1]^s\), and \(a\) is renormalized to satisfy the following condition:

\[ \sum_{i=1}^s a_i = h_j, \]

where \(h_j\) depends on the family \(f_j\). By varying \(a\) and \(u\), we formed quantitative examples based on 20 random samples for each function class. For any sample size \(|P| = 2^m\) and any function \(f_j\), we computed the median of the relative errors (in log10 scale)

\[ \log_{10} \frac{|I(f_j) - I_N(f_j)|}{|I(f_j)|} \]

varying the parameters, where \(I(f_j) := \int_{[0,1]^s} f_j \, dx\), \(N := |P|\), and \(I_N(f_j) := (1/|P|) \sum_{x \in P} f(x)\).
Figure 2 shows a summary of the medians of the relative errors for $s = 5$, $m = 1, \ldots, 23$, and $(h_1, \ldots, h_6) = (4.5, 3.625, 0.925, 3.515, 1.02, 2.15)$, which are the same settings in [11]. For $f_1$ and $f_3$, the low-WAFOM point sets are clearly superior to the Niederreiter-Xing nets. In particular, the scrambled Sobol’ nets represent a drastic improvement over the original Sobol’ nets. Note that the slopes are similar to those in Figure 1. Additionally, for $f_2$ and $f_4$, the low-WAFOM point sets are competitive with the Niederreiter–Xing nets. In these smooth functions, the WAFOM criterion seems to work very well. In the case of non-smooth functions, the situations is different. For the continuous but non-differentiable functions $f_5$, the naive low-WAFOM point sets are inferior to the Niederreiter–Xing nets. However, when we take into account the structure of $(t, m, s)$-nets, the low-WAFOM point sets preserve the rate of convergence. For $f_6$, the naive low-WAFOM point sets are also inferior to the other point sets with small $t$-values. These results imply that the structure of $(t, m, s)$-nets is important for non-smooth functions.

5. Conclusions and future directions

In this paper, we have searched for point sets whose $t$-value and WAFOM are both small so as to be effective for a wider range of function classes. For this, we fixed digital $(t, m, s)$-nets in advance and applied random linear scrambling. The key technique was to select linearly scrambled $(t, m, s)$-nets in terms of WAFOM. Numerical experiments showed that the point sets obtained by our method have improved convergence rates for smooth functions and are robust for non-smooth functions.

Finally, we discuss some directions for future research. In our approach, $m$ was fixed and the extensibility was discarded. We also attempted to search for extensible point sets, but the WAFOM values tend to be worse than the current ones for large $m$. Thus, an efficient search algorithm for extensible scrambling matrices is one area of future work. As another direction, the quasi-Monte Carlo method is an important tool in computational finance (e.g., [9, 13]). However, many applications encounter integrands with boundary singularities. Such integrands are not included in a suitable class of functions, i.e., $n$-smooth functions, so we might not expect higher order convergence from the simple application of low-WAFOM point sets. There will probably be a need for some kind of transformation to force the integrand to be included in a suitable class of functions, such as periodization.
Figure 2: Median of relative errors for Genz functions.
in lattice rules. The study of WAFOM is still in its infancy, so a number of unsolved problems remain.

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