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SCRAMBLING NON-UNIFORM NETS

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ABSTRACT. In this paper, we consider Owen's scrambling of an $(m-1, m, d)$-net in base b which consists of d copies of a $(0, m, 1)$-net in base b, and derive an exact formula for the gain coefficients of these nets. This formula leads us to a necessary and sufficient condition for scrambled $(m-1, m, d)$-nets to have smaller variance than simple Monte Carlo methods for the class of L_2 functions on $[0, 1]^d$. Secondly, from the viewpoint of the Latin hypercube scrambling, we compare scrambled non-uniform nets with scrambled uniform nets. An important consequence is that in the case of base two, many more gain coefficients are equal to zero in scrambled $(m-1, m, d)$-nets than in scrambled Sobol' points for practical size of samples and dimensions.

1. Introduction

In a recent paper [13], we considered a very narrow class of artificial functions for which scrambled $(m-1, m, d)$-nets in base two provide much smaller variance than simple Monte Carlo methods. In this paper, we analyze the variance of scrambled $(m-1, m, d)$-nets in general base b for the L_2 class of functions on $[0, 1]^d$. Historically speaking, Owen's scrambling ([5], [6], [7]) has an exact formula for the error variance of the integration with N points in terms of the scrambling. Although this formula is valid for any set of N points in $[0, 1)^d$, so far only the case of uniform or low-discrepancy points, in particular, (t, m, d)-nets or (t, d)-sequences ([4], [11]), has been intensively investigated (e.g., [2], [14]). The aim of this paper is to explore another application of Owen's scrambling, i.e., non-uniform points.

The organization of this paper is as follows: In Section 2, we overview Owen's scrambling and its formula for the variance of integration error. In Section 3,

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we consider the scrambling of an $(m-1, m, d)$-net in base b which consists of d copies of a $(0, m, 1)$-net in base b, and derive an exact formula for the gain coefficients of these nets. This formula leads us to a necessary and sufficient condition for scrambled $(m-1, m, d)$-nets to have smaller variance than simple Monte Carlo methods. In Section 4, from the viewpoint of the Latin hypercube scrambling, we compare scrambled non-uniform nets with scrambled uniform nets. An important consequence is that in the case of $b = 2$, much more gain coefficients are equal to zero in scrambled $(m-1, m, d)$-nets than in scrambled Sobol' points for practical size of samples and dimensions. In the last section, we discuss the significance of this result and future research directions.

2. Overview of Owen's scrambling

Owen's scrambling scheme is described as follows ([5], [6], [7]): 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 $A = a_1 b^{-1} + a_2 b^{-2} + \cdots$, where $a_1, a_2, \ldots$ are in $\{0, 1, \ldots, b-1\}$. Then the first b-ary digit of $\sigma(A)$ is $\pi(a_1)$, where π is a fixed permutation of the set $\{0, 1, \ldots, b-1\}$. Next, for each possible value of a_1, we fix a permutation π_{a_1} of $\{0, 1, \ldots, b-1\}$, 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 $\pi_{a_1,a_2}(a_3), \pi_{a_1,a_2,a_3}(a_4), \ldots$. In Owen's scrambling scheme, each permutation is uniformly distributed over the $b!$ possible permutations and the permutations are mutually independent. In d dimensions, we consider a d-tuple of b-ary scramblings $(\sigma_1, \ldots, \sigma_d)$. Owen showed that if $\sigma_1, \ldots, \sigma_d$ are chosen as fully random and mutually independent, then the d-dimensional scrambling keeps the t values of (t, m, d)-nets to be unchanged. Hereafter, we denote the d-dimensional integral by

$$\mathrm{I}(f) = \int\limits_{[0,1]^d} f(x_1, \ldots, x_d)\, \mathrm{d}x_1 \cdots \mathrm{d}x_d,$$

and the cubature using N points, $X_0, \ldots, X_{N-1} \in [0, 1)^d$, by

$$\mathrm{Q}_N(f) = \frac{1}{N} \sum_{n=0}^{N-1} f(X_n).$$

For the application of Owen's scrambling to high-dimensional integration, we should notice that for Owen's scrambling of any N point set in $[0, 1)^d$, the cubature becomes unbiased, i.e.,

$$\mathrm{E}(\mathrm{Q}_N(f)) = \mathrm{I}(f),$$

where the expectation is taken with respect to Owen's scrambling of the point set.

Owen [5], [6], [7] 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 $[0,1]^d$. First, we need recall the b-ary Haar wavelets on $[0,1)$:

$$\psi_{k,t,c}(x) = b^{\frac{k}{2}} \left(b1_{\lfloor b^{k+1}x \rfloor = bt+c} - 1_{\lfloor b^k x \rfloor = t} \right),$$

where k, t, c are integers with $k \geq 0$, $0 \leq t < b^k$, and $0 \leq c < b$. A function $f \in L_2[0,1]^d$ has the b-ary Haar wavelet expansion:

$$f(x_1, \ldots, x_d) = \mathrm{I}(f) + \sum_{\emptyset \neq u \subseteq \{1,\ldots,d\}} \sum_{\kappa} \sum_{\tau} \sum_{\gamma} \alpha_{u,\kappa,\tau,\gamma} \prod_{i \in u} \psi_{k_i,t_i,c_i}(x_i),$$

where κ, τ, and γ are vectors of $|u|$ elements k_i, t_i, and c_i for $i \in u$, respectively, and the coefficients are given by

$$\alpha_{u,\kappa,\tau,\gamma} = \int\limits_{[0,1)^d} f(x_1, \ldots, x_d) \prod_{i \in u} \psi_{k_i,t_i,c_i}(x_i) \, \mathrm{d}x_1 \ldots \mathrm{d}x_d.$$

Next, we define the following step function by

$$\nu_{u,\kappa}(x_1, \ldots, x_d) = \sum_{\tau} \sum_{\gamma} \alpha_{u,\kappa,\tau,\gamma} \prod_{i \in u} \psi_{k_i,t_i,c_i}(x_i),$$

which is constant within the subintervals

$$\prod_{i \in u} \left[\frac{j_i}{b^{k_i+1}}, \frac{j_i+1}{b^{k_i+1}} \right) \times \prod_{i \notin u} [0,1),$$

where $0 \leq j_i < b^{k_i+1}$ for $i \in u$. We should note that the class of functions considered in [13] is the one consisting only of $\nu_{u,\kappa}(x_1, \ldots, x_d)$ with κ satisfying that all k_i, $i \in u$, are identical.

Now, we recall the definition of gain coefficients $\Gamma_{u,\kappa}$. Denote a set of N points in $[0,1)^d$ by $X_n = \left(X_n^{(1)}, \ldots, X_n^{(d)}\right)$, $n = 0, \ldots, N-1$. Then, the gain coefficient is defined by

$$\Gamma_{u,\kappa} = \frac{1}{N(b-1)^{|u|}} \sum_{n=0}^{N-1} \sum_{n'=0}^{N-1} \prod_{i \in u} \left(b1_{\lfloor b^{k_i+1} X_n^{(i)} \rfloor = \lfloor b^{k_i+1} X_{n'}^{(i)} \rfloor} - 1_{\lfloor b^{k_i} X_n^{(i)} \rfloor = \lfloor b^{k_i} X_{n'}^{(i)} \rfloor} \right).$$

Owen obtained the following formula for the variance of the integration error in terms of his scrambling:

$$\mathrm{V}(f; N; X_n) \equiv \mathrm{E}\left[\left(\mathrm{Q}_N(f) - \mathrm{I}(f) \right)^2 \right] = \frac{1}{N} \sum_{u \neq \emptyset} \sum_{\kappa} \Gamma_{u,\kappa} \sigma_{u,\kappa}^2, \tag{1}$$

where $\sigma_{u,\kappa}^2$ is the variance of the step function $\nu_{u,\kappa}$.

We should note that the variance for simple Monte Carlo methods with N samples is

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

3. Analysis of scrambled non-uniform nets

Here, we apply Owen's scrambling to an $(m-1, m, d)$-net in base b which consists 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. By definition, a (t, m, d)-net is also a (u, m, d)-net for any $m \geq u > t$. The $(m-1, m, d)$-net considered in this paper is a strict $(m-1, m, d)$-net, i.e., it is not a (t, m, d)-net for $t < m-1$. This is why we call it a non-uniform net. As mentioned before, a scrambled $(m-1, m, d)$-net is again an $(m-1, m, d)$-net, and hence non-uniform. We remark that for some class of functions the property of having low-discrepancy is not a necessary condition for the speed-up of their numerical integration. For more details in this direction and the definition of high-discrepancy sequences, see Tezuka [12].

We prove the following theorem:

Theorem 1. *Let $\kappa = (k_, \dots, k_d)$, $u \subseteq \{1, \dots, d\}$, and $k_{\max} = \max_{i \in u} k_i$. Denote by $h(u, \kappa)$ the number of i such that $k_i = k_{\max}$. For Owen's scrambling of an $(m-1, m, d)$-net, 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*

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

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 equation (2), we obtain a necessary and sufficient condition for scrambled non-uniform nets to have a smaller variance than simple Monte Carlo methods as follows:

Corollary 1. *For the integration of an L_2 function on $[0, 1]^d$, scrambled $(m-1, m, d)$-nets in base b have smaller variance than simple Monte Carlo methods if and only if*

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

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

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

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

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. For the class of functions considered in [13], 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.

To prove Theorem 1, we use the next two lemmas:

Lemma 1. *Let A_n, $n = 0, \dots, N-1$, be N points in $[0, 1)$. Denote*

$$g_{n,n'}(k) = b 1_{\lfloor b^{k+1} A_n \rfloor = \lfloor b^{k+1} A_{n'} \rfloor} - 1_{\lfloor b^k A_n \rfloor = \lfloor b^k A_{n'} \rfloor}$$

for integers $0 \leq n, n' \leq N-1$ and $k \geq 0$. The following statements hold:

- *If there exists some k such that $g_{n,n'}(k) = b-1$, then $g_{n,n'}(k+1) = b-1$ or -1.*
- *If there exists some k such that $g_{n,n'}(k) = -1$, then $g_{n,n'}(k+1) = 0$.*
- *If there exists some k such that $g_{n,n'}(k) = 0$, then $g_{n,n'}(k+1) = 0$.*

Proof. For any $k \geq 0$, if $\lfloor b^k A_n \rfloor \neq \lfloor b^k A_{n'} \rfloor$, then $\lfloor b^{k+1} A_n \rfloor \neq \lfloor b^{k+1} A_{n'} \rfloor$. Thus, $g_{n,n'}(k)$ takes only three values, -1, 0, and $b-1$. The proof immediately follows. □

Lemma 2. *If A_n, $n = 0, \dots, b^m - 1$, is a $(0, m, 1)$-net in base b, then for $0 \leq k \leq m-1$,*

- *the number of pairs (n, n') such that $g_{n,n'}(k) = b-1$ is b^{2m-k-1}, and*
- *the number of pairs (n, n') such that $g_{n,n'}(k) = -1$ is $(b-1)b^{2m-k-1}$.*

For $k \geq m$, $g_{n,n'}(k) = 0$ for all pairs (n, n') except for $n = n'$, for which $g_{n,n}(k) = b-1$.

Proof. The proof follows directly from the definition of $(0, m, 1)$-nets. □

Proof of Theorem 1. According to Lemma 1, if $k_{\max} < m$, we have, for any pair (n, n') with $0 \leq n, n' \leq N-1$,

$$\begin{aligned}
\prod_{i \in u} g_{n,n'}(k_i) &= \prod_{i \in u} \Big(b 1_{\lfloor b^{k_i+1} X_n^{(i)} \rfloor = \lfloor b^{k_i+1} X_{n'}^{(i)} \rfloor} - 1_{\lfloor b^{k_i} X_n^{(i)} \rfloor = \lfloor b^{k_i} X_{n'}^{(i)} \rfloor} \Big) \\
&= \begin{cases} (b-1)^{|u|} & \text{if } g_{n,n'}(k_{\max}) = b-1, \\ (-1)^{h(u,\kappa)} (b-1)^{|u|-h(u,\kappa)} & \text{if } g_{n,n'}(k_{\max}) = -1, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

Therefore, from the first half of Lemma 2, we have

$$\Gamma_{u,\kappa} = \frac{1}{b^m(b-1)^{|u|}} \sum_{n=0}^{b^m-1} \sum_{n'=0}^{b^m-1} \prod_{i \in u} g_{n,n'}(k_i) = b^{\ell(u,\kappa)} \left(1 + \frac{(-1)^{h(u,\kappa)}}{(b-1)^{h(u,\kappa)-1}}\right),$$

if $k_{\max} < m$. For the case $k_{\max} \geq m$, we have

$$\Gamma_{u,\kappa} = 1,$$

due to the second half of Lemma 2. Thus, the proof is complete. □

4. Connection with Latin hypercube sampling

In this section, we discuss scrambled non-uniform nets introduced in this paper from the viewpoint of the Latin hypercube sampling (LHS), which is defined as follows ([3], [5]):

Definition 1. Let $p_1, \ldots, p_d$ be randomly chosen independent permutations over $\{0, 1, \ldots, N-1\}$. A *Latin hypercube sampling of N points* is given by

$$\left(\frac{p_1(i) + U_i^{(1)}}{N}, \ldots, \frac{p_d(i) + U_i^{(d)}}{N}\right), \qquad i = 0, 1, \ldots, N-1,$$

where $U_i^{(j)}$, $j = 1, \ldots, d$, $i = 0, 1, \ldots, N-1$, are independent random variables uniformly distributed in $[0, 1)$.

Since Theorem 1 implies that the case of $b = 2$ is the most interesting and useful one for practical applications, hereafter we assume that $b = 2$, $m > 1$, and $N = 2^m$. The most important property of LHS for numerical integration is that LHS has nearly no errors and thus better than simple Monte Carlo if an integrand is additive functions of the form $\sum_{i=1}^{d} f_i(x_i)$ and N is large, in other words, LHS has zero gain coefficients for $|u| = 1$ and small κ. According to Theorem 1, when $|u| = 1$, we always have $\Gamma_{u,\kappa} = 0$ if $k_i < m$ for $i \in u$. Thus, scrambled non-uniform nets also have the same advantage as LHS if the dominant part of an integrand is additive functions.

We denote by $\mathscr{L}$ the set of all Latin hypercube samples of 2^m points. Let P be a set of 2^m points in $[0, 1)^d$. We denote by $\mathscr{L}_P$ the set of all nets obtained by applying Owen's scrambling to P. If P is an $(m-1, m, d)$-net in base 2 which consists of d copies of a $(0, m, 1)$-net in base 2, $\mathscr{L}_P$ is a proper subset of $\mathscr{L}$, since each coordinate of P is a $(0, m, 1)$-net. If P is Sobol' points of length 2^m, $\mathscr{L}_P$ is another proper subset of $\mathscr{L}$, since each coordinate of Sobol' points is a $(0, m, 1)$-net. Thus, we will compare these two different proper subsets of $\mathscr{L}$, i.e., non-uniform nets vs. uniform nets. Since the gain coefficients of Sobol' points depend on the choice of direction numbers, we use Sobol' Property A, which has been recently adopted in practice ([1], [9]) to determine direction numbers. The definition of Property A is as follows:

Definition 2. An m-dimensional sequence $X_0, X_1, \dots,$ is said to satisfy *Sobol' Property A* if for every $j = 0, 1, \dots,$ exactly one of points X_n, $j2^m \le n < (j+1)2^m$, fall in each of the 2^m cubes of the form $\prod_{i=1}^{m} \left[\frac{a_i}{2}, \frac{a_i+1}{2}\right)$, where $a_i = 0$ or 1.

More precisely, here we consider a d-dimensional Sobol' sequence $X_0, X_1, \dots,$ such that all of its m-dimensional projections satisfy Property A, where we assume $m \le d$. Note that any segment X_n, $j2^m \le n < (j+1)2^m$, of the Sobol' sequence has $\Gamma_{u,\kappa} = 1$ either when $k_{\max} \ge m$ or when $|u| \ge m$.

For the comparison, as a rule of thumb, we use the number of gain coefficients which are equal to zero. Since when $k_{\max} \ge m$, $\Gamma_{u,\kappa} = 1$ also for scrambled $(m-1, m, d)$-nets, the comparison should be done for the case $k_{\max} < m$. As already shown, for scrambled $(m-1, m, d)$-nets, half of the gain coefficients are equal to zero when $|u| \le d$. On the other hand, for scrambled Sobol' points, $\Gamma_{u,\kappa} = 1$ when all $|u| \ge m$ regardless of $k_{\max}$, and $\Gamma_{u,\kappa} = 0$ when both $|u|$ and $k_{\max}$ are small. In other words, when $m \le |u| \le d$ scrambled Sobol' points have no gain coefficients which are zero. This difference is remarkable for practical applications in which d is sometimes as large as 100 or more, and m is as large as 10 to 20. The known upper bound of gain coefficients for scrambled Sobol' points is $2^{t+|u|-1}$, see [7], where the value of t is known to be the order of $d \log d$ ([8]). On the other hand, the maximum of the gain coefficients for scrambled $(m-1, m, d)$-nets is 2^m, which is much smaller than 2^d in practical applications.

5. Discussion

Asymptotically, as $N \to \infty$, the error variance goes to zero for the case of scrambled QMC. However, in practice of scrambled QMC we use a fixed N, and by using independent M repetitions of the scrambling we estimate the variance. On the other hand, we have no guarantee for the asymptotic convergence of scrambled non-uniform nets, although for some special class of functions we can prove the $O(N^{-1})$ convergence rate of (deterministic) high-discrepancy sequences ([12]). But, in the same way as scrambled QMC, for a fixed N, we can estimate the error variance for scrambled non-uniform nets by using M independent repetitions of the scrambling. Thus, according to the central limit theorem, as $M \to \infty$, the error goes to zero also for scrambled non-uniform nets as well as scrambled QMC.

An important point from our results is that Owen's scrambling works well with not only low-discrepancy (or uniform) points but also non-uniform points. Owen's formula (1) corresponds to Hlawka-Sobol'-Zaremba's identity ([10]) for QMC, where the gain coefficient is to the function variance as the local discrepancy is to the function variation. However, as shown in [13], the gain coefficient is not necessarily a measure of high-dimensional uniformity of points due to its product structure. This makes scrambled non-uniform points useful for some high-dimensional problems.

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