Secure pseudorandom bit generators and point sets with low star-discrepancy

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Abstract

The star-discrepancy is a quantitative measure for the irregularity of distribution of a point set in the unit cube that is intimately linked to the integration error of quasi-Monte Carlo algorithms. These popular integration rules are nowadays also applied to very high-dimensional integration problems. Hence multi-dimensional point sets of reasonable size with low discrepancy are badly needed. A seminal result from Heinrich, Novak, Wasilkowski and Woźniakowski shows the existence of a positive number C such that for every dimension d there exists an N-element point set in $[0,1)^d$ with star-discrepancy of at most $C\sqrt{d/N}$. This is a pure existence result and explicit constructions of such point sets would be very desirable. The proofs are based on random samples of N-element point sets which are difficult to realize for practical applications.

In this paper we propose to use secure pseudorandom bit generators for the generation of point sets with star-discrepancy of order $O(\sqrt{d/N})$. This proposal is supported theoretically and by means of numerical experiments.

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1. Introduction

Let $d, N \in \mathbb{N}$. For an N-element point set $\mathcal{P} = \{x_1, \dots, x_N\}$ in the d-dimensional unit-cube $[0, 1)^d$ the star-discrepancy is defined as

$$D_N^*(\mathcal{P}) = \sup_{\boldsymbol{t} \in [0,1]^d} \left| \frac{\#\{k \in \{1,\ldots,N\} : \boldsymbol{x}_k \in [\boldsymbol{0},\boldsymbol{t})\}}{N} - \text{volume}([\boldsymbol{0},\boldsymbol{t})) \right|,$$

where, for $\mathbf{t} = (t_1, \dots, t_d) \in [0, 1]^d$, $[\mathbf{0}, \mathbf{t}) = [0, t_1) \times \dots \times [0, t_d)$. The star-discrepancy is a quantitative measure for the irregularity of distribution which is closely related to the integration error of quasi-Monte Carlo (QMC) rules via the well-known Koksma-Hlawka inequality (see [6, 18, 20, 22]). Traditionally this has found application to different domains such as option pricing, experimental design or antialiasing techniques in computer graphics.

Classically, the star-discrepancy is studied in an asymptotic setting for a fixed dimension d when N tends to infinity. The best results in this context are point sets with star-discrepancy of order of magnitude $O((\log N)^{d-1}/N)$. Often it is conjectured, that this order of magnitude is the best what one can achieve in dimension d. This is a still open question but it must be confessed that there are also other opinions (c.f. [5]).

However, in practical applications of QMC methods the dimension d can be very large and in this regime an error bound of order $O((\log N)^{d-1}/N)$ is useless for point sets of manageable size N. Consider, for example, a point set with $N=2^d$ elements, which is already very large when $d\geq 25$ (in applications dimension d might be in the hundreds or thousands). Then, $(\log N)^{d-1}/N \approx d^{d-1}/2^d$ which demonstrates how useless the asymptotic excellent discrepancy bounds are for practical problems. Larcher [19] was the first to create doubts whether a star-discrepancy bound of asymptotically excellent order can help for practical applications.

From late 1990s this problem has attracted a lot interest, see for example the surveys in [23, Section 3.1.5] and [24, Section 9.9] and the references therein. It is now known that there exists some C > 0 such that for every N and d there exists an N-element point set \mathcal{P} in $[0,1)^d$ whose star-discrepancy

satisfies

$$D_N^*(\mathcal{P}) \le C\sqrt{\frac{d}{N}}. (1)$$

This is a famous result by Heinrich, Novak, Wasilkowski and Woźniakowski [16]. Aistleitner [1] proved that C can be chosen to be 10 and very recently, Gnewuch and Hebbinghaus [13] reduced C further to the value 2.5287... The proofs of these results are based on the fact that the expected star-discrepancy of a randomly generated point set satisfies the inequality in (1). However, as Aistleitner and Hofer pointed out in [2], such a mere existence result is not of much use for applications. Furthermore, they proved a version of (1) which provides estimates for the probability of a random point set to satisfy it. Their results demonstrate that the probability q, that a random point set satisfies a star-discrepancy bound of the form $c(q, d) \sqrt{d/N}$, is extremely large already for moderate values of c(q, d) (see the forthcoming Lemma 2).

A straightforward approach is to simply choose a random sample of N uniformly i.i.d. points in $[0,1)^d$ and then one can assume, with very large probability, that the star-discrepancy of this sample is sufficiently small. This has not being met with general acceptance due to three main shortcomings:

- First, the computation of the star-discrepancy of a given multi-dimensional point set is very difficult (see, e.g., [14]). So even for moderate values of d it is almost impossible the check whether the obtained random sample is really of low star-discrepancy.
- Second, it is possible to use some heuristic to approximate the discrepancy and search for good candidates. There have been studies for searching for good point sets using known constructions. Doerr and De Rainville [9] considered generalized Halton sequences and tried to identify good permutations for them. Although the computer experiments are promising, the nature of the work is heuristic.
- The next problem, which we address in the present work, is how to efficiently generate random samples on a computer from uniformly i.i.d. random variables in $[0,1)^d$.

Pseudorandom number generators are any kind of algorithms that generate a sequence of numbers with similar properties to random sequences of numbers. Special classes of pseudorandom number sequences have been proved to be of low star-discrepancy using the Erdös-Turan inequality. Even

that this approach is useful for certain applications, i.e to prove normality of specific real numbers (see [3]), the obtained discrepancy bounds depend exponentially on the dimension. Our approach is to replace random samples by point sets obtained from secure pseudorandom bit generators. The employed pseudorandom bit generator requires as input a finite string of bits called seed, then the sequence of pseudorandom bits is transformed in a natural way to a point set in the unit-cube $[0,1)^d$ with prescribed p bits of precision. Under the assumption of uniformly chosen seed we show that the obtained point sets satisfy the desired discrepancy bound of order $\sqrt{d/N}$ with high probability. Our proposed method is supported by numerical results up to dimension d=15. These results also support a conjecture by Novak and Woźniakowski [24, p. 68].

We remark that obviously also our approach is not fully constructive. Still we need a random seed for the present construction based on pseudorandom bit generators, even if this is in a way "less" random compared for example with the approach in [16].

The paper is organized as follows: In Section 2 we provide the necessary material related to secure pseudorandom bit generators and the construction of the point sets. Section 3 is devoted to the theoretical result which guarantees for reasonable values of d and N that the proposed point sets have discrepancy of order $\sqrt{d/N}$ with high probability when the seed is i.i.d. uniformly distributed. In Section 4 we present numerical results which support the proposed use of secure pseudorandom bit generators for the construction of point sets with low star-discrepancy.

2. Secure pseudorandom bit generators and point sets in the unit cube

This section provides the basic notation that we will employ through the paper. A binary word is a string of bits, i.e. of zeros and ones. The set with binary words of length n is denoted by $\{0,1\}^n$. A uniformly distributed random variable on $\{0,1\}^n$ is denoted by U_n . We remark that the index n always refers to the length of the binary words.

Definition 1. Let $m, n \in \mathbb{N}$, where usually n is much smaller than m. A pseudorandom bit generator is a function $f : \{0,1\}^n \to \{0,1\}^m$, which can be evaluated efficiently. Modern implementations can generate up to 113.5 Gigabits per seconds of random bits [12].

The *seed* or input of a pseudorandom bit generator is a binary word of length n. It is assumed that the seed is based on true random information. The output is a pseudorandom bit sequence of length m.

To define a secure pseudorandom bit generator, we use the notion of a (T, ε) -distinguisher (see [11]).

Definition 2. Let $T \in \mathbb{N}$ and $\varepsilon > 0$. A (T, ε) -distinguisher for a pseudorandom bit generator f is any probabilistic algorithm \mathcal{D} whose input are binary words of length m and which returns, after at most T time units, a value of 0 or 1 such that

$$|\mathbb{P}[\mathcal{D}(f(U_n)) = 1] - \mathbb{P}[\mathcal{D}(U_m) = 1]| \ge \varepsilon.$$

Then, a pseudorandom number generator f is said to be (T, ε) -indistinguishable if no (T, ε) -distinguisher exists for f.

A pseudorandom number generator f is said to have b bits of security if every (T, ε) -distinguisher for f satisfies

$$T > 2^b \varepsilon^2$$
:

see [21] for further reading. Equivalently, for a pseudorandom number generator f with b bits of security, any probabilistic algorithm \mathcal{D} with run time of at most T time units that returns a value of 0 or 1 for any input sequence from $\{0,1\}^m$, we have

$$|\mathbb{P}[\mathcal{D}(f(U_n)) = 1] - \mathbb{P}[\mathcal{D}(U_m) = 1]| < \sqrt{\frac{T}{2^b}}.$$
 (2)

To initialize a pseudorandom bit generator a seed of n bits must be provided that supports the security strength b requested by the implementation of the generator mechanism. For example, a Hash-pseudorandom bit generator based on SHA-512 has parameters n=888 for b=256, see [4, p. 38, Table 2]. Constructions of pseudorandom number generators that achieve at least b bits security are known for any b (see, e.g., [15]) but only the cases $b \in \{112, 128, 192, 256\}$ are standardized (see, e.g., [4]). We note that this holds for any practical value of m.

Transforming binary words to point sets in the unit cube. To convert a binary word of length m to a N-element point set in $[0,1)^d$ we use the following binary interchange format: For a given precision $p \in \mathbb{N}$, take the p trailing significant field string represented by a binary word d_1, d_2, \ldots, d_p , then

$$\sum_{i=1}^{p} \frac{d_i}{2^i}$$

is a coordinate of an element of the point set \mathcal{P} . For p=52, this representation follows the double-precision floating-point format binary64, see [17].

For a given binary word U_m we denote the resulting point set by $\mathcal{P}(U_m)$, in this case we will require m = pdN bits to construct N points in $[0, 1)^d$.

3. Theoretical results on star-discrepancy for pseudorandom point sets

We consider a particular distinguisher \mathcal{D} which takes a binary word U_m of length m, generates a sequence of points $\mathcal{P} = \mathcal{P}(U_m) = \{X_1, \ldots, X_N\}$ in the d dimensional unit cube $[0,1)^d$ as described above and calculates the star-discrepancy of \mathcal{P} . The distinguisher returns 1 if the star-discrepancy is greater than $C\sqrt{d/N}$, where C is a suitably chosen constant. The star-discrepancy of an N-element point set in $[0,1)^d$ can be calculated in $O(N^{1+d/2})$ operations (see [7, 10, 14]).

In order to generate the binary words U_m we use a pseudorandom bit generator

$$f: \{0,1\}^n \to \{0,1\}^m$$

with b bits of security, which will be explicitly selected later. We note that n is much smaller than m = pdN, in our applications p = 52, i.e., m = 52dN.

Theorem 1. Let $n, p, d, N \in \mathbb{N}$ and let m = pdN. Assume that $f(U_n)$ is obtained from a pseudorandom bit generator $f : \{0, 1\}^n \to \{0, 1\}^m$ with b bits of security. Let $\mathcal{P}(f(U_n))$ be the corresponding N-element point set in $[0, 1)^d$ with random seed U_n . Then we have

$$\mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}}\right]$$

$$\le \exp\left(4.9 - \frac{1}{5.7^2}\left(C - \frac{\sqrt{dN}}{2^p}\right)^2\right) + O\left(\sqrt{\frac{N^{1+d/2}}{2^b}}\right).$$

For a choice of values of bit security b=256 and precision p=52, the bound on the probability in Theorem 1 is very small for reasonable values of d and N whenever $C>\sqrt{4.9}\cdot 5.7=12.6174\ldots$ To be more precise, with these values for p and b the above bound on the probability is essentially $\exp(4.9-(C/5.7)^2)=:g(C)$ as long as $N^{1+d/2}\ll 2^{256}$. We have the following (rounded) values:

For the proof of Theorem 1 we need the following lemmas.

Lemma 1. Let X_1, \ldots, X_N be uniformly i.i.d. in $[0,1)^d$ with $X_j = (X_{j,1}, \ldots, X_{j,d})$ for $j \in \{1, \ldots, N\}$. For $p \in \mathbb{N}$ and $i \in \{1, \ldots, d\}$ let

$$X_{j,i}^{(p)} := \frac{\lfloor 2^p X_{j,i} \rfloor}{2^p} \in \left\{ 0, \frac{1}{2^p}, \dots, \frac{2^p - 1}{2^p} \right\} \quad and \quad X_j^{(p)} = (X_{j,1}^{(p)}, \dots, X_{j,d}^{(p)}).$$

Consider the binary expansion of $X_{j,i}^{(p)}$ and concatenate the corresponding dN binary words to obtain a binary word U_m of length m = pdN. Then

- 1. $\mathcal{P}(U_m) = \{X_1^{(p)}, \dots, X_N^{(p)}\};$
- 2. U_m is uniformly distributed in $\{0,1\}^m$;
- 3. the star-discrepancies of $\mathcal{P} = \{X_1, \dots, X_N\}$ and $\mathcal{P}(U_m)$ differ at most by $d/2^p$, i.e.,

$$|D_N^*(\mathcal{P}) - D_N^*(\mathcal{P}(U_m))| \le \frac{d}{2^p}; \tag{3}$$

4. for C > 0 we have

$$\mathbb{P}\left[D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}}\right] \le \mathbb{P}\left[D_N^*(\mathcal{P}) \ge C\sqrt{\frac{d}{N}} - \frac{d}{2^p}\right]. \tag{4}$$

Proof. Items 1. and 2. are obviously true. In order to prove 3. note first that for every $j \in \{1, ..., N\}$ we have

$$||X_j - X_j^{(p)}||_{\infty} \le \frac{1}{2^p},$$

where $\|\cdot\|_{\infty}$ denotes the ℓ_{∞} -norm in \mathbb{R}^d . Therefore (3) follows from [6, Proposition 3.15]. Finally we show 4. For C > 0 we obtain from (3) that

$$D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}} \implies D_N^*(\mathcal{P}) \ge C\sqrt{\frac{d}{N}} - \frac{d}{2^p}$$

and hence we obtain (4).

The following result is [2, Corollary 1].

Lemma 2 (Aistleitner and Hofer). For any $d, N \in \mathbb{N}$ and $q \in (0,1)$ a randomly generated d-dimensional point set \mathcal{P} in $[0,1)^d$ satisfies

$$D_N^*(\mathcal{P}) \le 5.7\sqrt{4.9 + \log((1-q)^{-1})}\sqrt{\frac{d}{N}}$$

with probability at least q.

Now we can state the proof of Theorem 1.

Proof of Theorem 1. Let \mathcal{P} be a set of uniformly i.i.d. points in $[0,1)^d$ and let $\mathcal{P}(U_m)$ be constructed as in the statement of Lemma 1. Then we have

$$\mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}}\right] \\
\le \mathbb{P}\left[D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}}\right] \\
+ \left|\mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}}\right] - \mathbb{P}\left[D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}}\right]\right|.$$

The first term can be bounded using Lemma 1 and Lemma 2. In particular, choosing q such that

$$5.7\sqrt{4.9 + \log((1-q)^{-1})}\sqrt{\frac{d}{N}} = C\sqrt{\frac{d}{N}} - \frac{d}{2^p}$$

we get

$$\mathbb{P}\left[D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}}\right] \le e^{4.9 - \frac{1}{5.7^2} \left(C - \frac{\sqrt{dN}}{2^p}\right)^2}.$$
 (5)

The second term can be bounded using Eq. (2) and the fact that the stardiscrepancy can be calculated in $O(N^{1+d/2})$ operations (see [7, 10]). This way we obtain

$$\left| \mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}} \right] - \mathbb{P}\left[D_N^*(\mathcal{P}(U_m)) \ge C\sqrt{\frac{d}{N}} \right] \right| < O\left(\sqrt{\frac{N^{1+d/2}}{2^b}}\right).$$

Together we obtain

$$\mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}}\right] \le e^{4.9 - \frac{1}{5.7^2} \left(C - \frac{\sqrt{dN}}{2^p}\right)^2} + O\left(\sqrt{\frac{N^{1+d/2}}{2^b}}\right).$$

Denoting ld the binary logarithm and choosing $b = \lceil 2 \operatorname{ld} C + \frac{d}{2} \operatorname{ld} N \rceil$ in Theorem 1 we obtain the following corollary:

Corollary 1. With the notation from Theorem 1 and with $b = \lceil 2 \operatorname{ld} C + \frac{d}{2} \operatorname{ld} N \rceil$ we obtain

$$\mathbb{P}\left[D_N^*(\mathcal{P}(f(U_n))) \ge C\sqrt{\frac{d}{N}}\right] \le O\left(\frac{1}{C^2}\right).$$

4. Numerical experiments

In order to support our approach, we have performed several numerical experiments during 83 days in one node (332.8 GFLOPS) of Altamira, the High Performance Computer cluster at the University of Cantabria. Altamira belongs to RES (Red Española de Supercomputación) network.

We generated a file with 40.000 hexadecimal digits with the library Openssl [25], using the default AES-256 CTR_DRBG with security bit strength b = 256. In this configuration, the required seed length is n = 384 bits in which at least 256 bits are supposed to be random and independent. The implementation employs entropy sources available to the computer (keystrokes, mouse movements, internal clock,...).

These hexadecimal bits are transformed into floating point numbers of precision p=52 and then, depending of the dimension, grouped in d-dimensional vectors following the steps described in Section 2. Finally the star-discrepancy is computed using the implementation of the algorithm by Dobkin, Eppstein and Mitchell [7] provided by Magnus Wahlström [26].

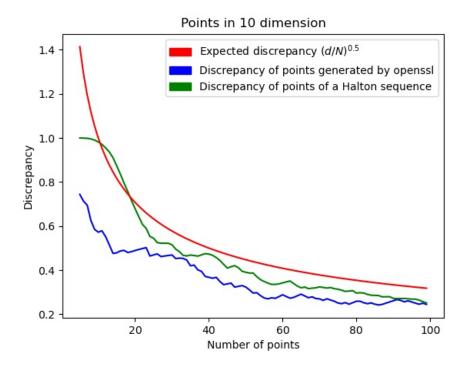


Figure 1: Discrepancy of N points in $[0,1)^{10}$, comparing with a Halton sequence where the bases are the first 10 primes.

First we present a comparison between the points generated and a Halton sequence for dimension d = 10, see Figure 1. The discrepancy of the generated points (plotted in blue) is always smaller than the one corresponding to the Halton sequence (plotted in green).

Further we present more results for the proposed point sequences in dimensions $d \in \{13, 14, 15\}$, which are displayed in Figures 2 - 4. The real values plotted in blue are compared with the graph of the bound $\sqrt{d/N}$ plotted in red.

We are also interested in the *inverse of star-discrepancy*, which is for given $\varepsilon \in (0,1)$ and dimension d the smallest size N of a point set in $[0,1)^d$ with star-discrepancy at most ε , i.e.,

$$N(\varepsilon,d) = \min\{N \in \mathbb{N} \ : \ \exists \mathcal{P} \subseteq [0,1)^d \ \text{ such that } |\mathcal{P}| = N \text{ and } D_N^*(\mathcal{P}) \leq \varepsilon\}.$$

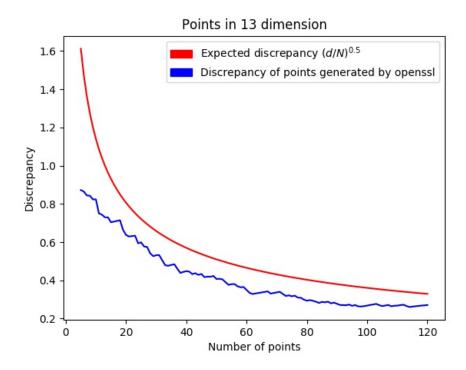


Figure 2: Discrepancy of N points in $[0,1)^{13}$

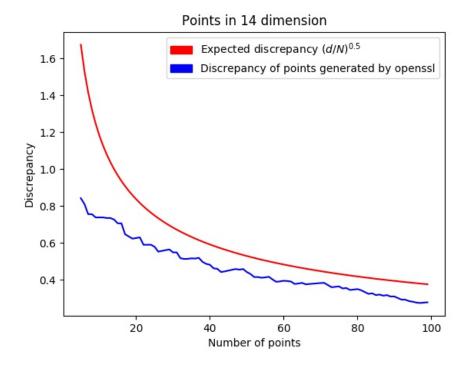


Figure 3: Discrepancy of N points in $[0,1)^{14}$

Note that (1) implies that

$$N(\varepsilon, d) \le C^2 d\varepsilon^{-2}$$
.

This means in the language of IBC (information based complexity) that the star-discrepancy is *polynomially tractable*.

Results on $N(\varepsilon, d)$ based on the proposed construction in this paper for $d \in \{2, 3, ..., 15\}$ and $\varepsilon \in \{0.5, 0.333, 0.25, 0.125\}$ are displayed in Table 1. Based on results in [8] for d < 10 it is conjectured by Novak and Woźniakowski in [24, p. 68] that N = 10d points in $[0, 1)^d$ suffice in order to achieve a star-discrepancy of at most 0.25. Our values N(0.25, d) from Table 1 are in this conjectured regime.

Finally, in Figure 5 we visualize two point sets in the two-dimensional cube. The one on the left hand side consists of 11 points and has star-discrepancy not larger than 0.25. The point set on the right hand side consists of 242 points and has star-discrepancy not larger than 0.1.

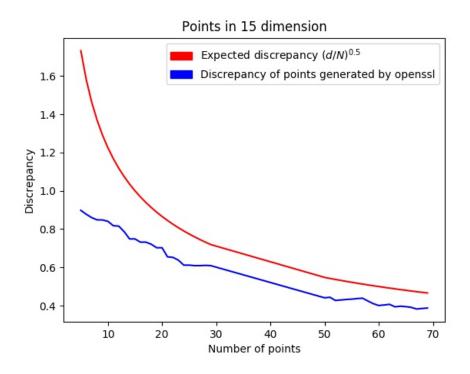


Figure 4: Discrepancy of N points in $[0,1)^{15}$

d	2	3	4	5	6	7	8	9	10	11	12	13	14	15	ε
$N(\varepsilon,d)$	10	13	10	25	26	24	28	31	14	30	32	33	38	50	0.5
$N(\varepsilon,d)$	10	45	36	55	60	52	62	61	47	70	75	62	83	-	0.333
$N(\varepsilon,d)$	11	87	78	93	82	76	96	94	76	108	120	-	-	-	0.25
$N(\varepsilon,d)$	215	195	194	232	214	325	304	-	-	-	-	-	-	-	0.125

Table 1: Dimension d versus $N(\varepsilon, d)$, the number of points generated using AES-256 CTR_DRBG necessary to reach a discrepancy of at most ε , for $\varepsilon \in \{0.125, 0.25, 0.333, 0.5\}$

5. Conclusions

In this work, we employed secure pseudorandom bit generators for the generation of point sets in $[0,1)^d$ of reasonable size with low star-discrepancy. The expected probability of obtaining point sets with star-discrepancy of order $C\sqrt{d/N}$ for specific parameters were given in Theorem 1. Previous

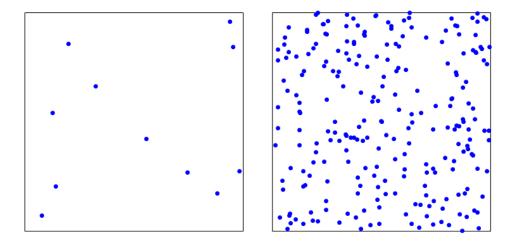


Figure 5: Point sets in $[0,1)^2$ with star-discrepancy less than 0.25 (11 points, left picture) and less than 0.1 (242 points, right picture)

theoretical results were pessimistic with respect to the value of the constant C whereas our numerical results suggest that the practical values are closer to 1. We hope that this study provides new insight into the problem of generating low discrepancy multidimensional point sets.

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