

Low Discrepancy Sequences

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February 18, 2016

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Implementation of the Low Discrepancy Sequences QMC simulation

Quasi Monte Carlo simulation consists in approximating the integral $\int_{[0,1]^d} f(u) du$ by $\frac{1}{N} \sum_{i=1}^N f(u_i)$ where $\{\xi_i\}$ are quasi-random numbers, that means they are generated from low-discrepancy sequences. As we already have explained it, such sequences neither are random nor pseudo-random but

deterministic and successive values are not independent. However they satisfy good properties of equidistribution on $[0, 1]^d$ and we have that $\frac{1}{N} \sum_{i=1}^N f(\xi_i) \rightarrow \int_{[0,1]^d} f(u) du$.

In the following sections we describe some low discrepancy sequences. We explain their construction and discuss some of their properties, especially on their discrepancy.

General references about the Quasi-Monte Carlo simulation are [2], [7], [8], [6] or [4].

The implementation of the sequences are described in [the implemented part](#).

1 Tore-SQRT sequences

They are d -dimensional sequences, obtained by considering the multiples of suitable irrational numbers modulo 1.

• Tore sequence

It is defined by :

$$\xi_n = (\{n.\alpha\}) = (\{n.\alpha_1\}, \dots, \{n.\alpha_d\})$$

where $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{R}^d$ such that $(1, \alpha_1, \dots, \alpha_d)$ are linearly independent on \mathbb{Q} .

$\{x\} = x - [x]$ denotes the fractional part of x .

• SQRT sequence

It is a particular case of the Tore sequence with

$$\alpha = (\sqrt{p_1}, \dots, \sqrt{p_d})$$

where (p_1, \dots, p_d) are the first d prime numbers.

If $\alpha_1, \dots, \alpha_d$ are algebraic, then the discrepancy satisfies:

$$D_n^*(\xi) = O\left(\frac{1}{n^{1-\varepsilon}}\right), \forall \varepsilon > 0$$

Click there to reach the implemented part: [implementation](#).

2 Van der Corput and Halton sequences

2.1 Van der Corput sequence

This is a one-dimensional sequence defined by the *radical-inverse function* φ_p in base p :

$$\varphi_p(n) = \sum_{i=0}^{R(n)} \frac{a_i}{p^{i+1}}$$

where the coefficients a_i are given by the digit expansion in base p of n :

$$n = \sum_{i=0}^{R(n)} a_i p^i$$

$R(n)$ denotes the maximum index for which $a_{R(n)}$ is not equals to 0. Its value depends on n and p by the relation $p^{R(n)} \leq n < p^{R(n)+1}$, that is:

$$R(n) = \left\lceil \frac{\log n}{\log p} \right\rceil$$

Discrepancy of the Van der Corput sequence satisfies the following majoration:

$$D_n^*(\xi) \leq \frac{1}{n} \frac{p \log(pn)}{\log(p)} = O\left(\frac{\log n}{n}\right)$$

Remarks: (ref Article of Alan Jung and Silvio Galanti)

- For $n < p$, there is only one positive coefficient a in the decomposition in base p , that is $a_0 = n$. Thus $\varphi_p(n) = \frac{n}{p}$ and the sequence is increasing.
- There are cycles of length p in this sequence. Each subsequence of length p (indices kp to $(k+1)p - 1$) is increasing in magnitude proportionnaly to power of $1/p$, and covers uniformly the interval $[0, 1)$. Consequences of this property will be studied for multidimensional sequences (especially Halton sequence).

2.2 Halton sequence

The Halton sequence is a d -dimensional generalization of the Van Der Corput sequence. Let (p_1, \dots, p_d) be the d first prime numbers, then ξ_n is defined by:

$$\xi_n = (\varphi_{p_1}(n), \dots, \varphi_{p_d}(n))$$

where $\varphi_{p_i}(n)$ is the Van der Corput sequence in base p_i .
The Halton sequence satisfies :

$$D_n^*(\xi) \leq \frac{1}{n} \prod_{i=1}^d \frac{p_i \log(p_i n)}{\log(p_i)} = O\left(\frac{\log^d(n)}{n}\right)$$

with a constant $C^d = \prod_{k=1}^d \frac{p_k - 1}{2 \log p_k}$.

This constant grows to infinity super-exponentially with dimension.

Click there to reach the implemented part: [implementation](#).

2.3 Permuted (Generalized) Halton sequence

Orthogonal projections of points from the Halton sequence show non uniform distribution for some dimensions (see Morokoff and Caflish [6], Jung ??? or Bratley and Fox ???). This non-uniformity is due to cycles of length p_i for each one-dimensional sequence.

To break correlations between the inverse radical functions of different dimensions, we realize permutations of coefficients a_i .

We consider $(\Pi_{p_i}, 1 \leq i \leq d)$ d permutations over $\{0, \dots, p_i - 1\}$ such that $\Pi_{p_i}(0) = 0$.

Each term of the *permuted Halton sequence* is defined by:

$$S_{p_i}(n) = \frac{\Pi_{p_i}(a_0)}{p_i} + \dots + \frac{\Pi_{p_i}(a_{R(n)})}{p_i^{R(n)+1}}$$

with $n = \sum_{i=0}^{R(n)} a_i p^i$.

The global sequence is given by :

$$\xi_n = (S_{p_1}(n), \dots, S_{p_d}(n))$$

There is no optimal choice for the permutations. We present 3 approaches to modify the Halton sequence

- An algorithm was suggested by Braaten and Weller [1] for $d \leq 16$ with a possible extension to a larger d (however with significant computation).

- Reverse-Radix Algorithm

An other algorithm (see Kocis and Whiten [5]) consists in reversing the binary digits of integers, expressed using a fixed number of base 2 digits and removing any values that are too large.

This algorithm can be applied for very large values of dimensions.

- Halton Sequence Leaped:

This other variant for the Halton sequence consists in using only every L th Halton number subject to the condition that L is a prime different from all bases p_1, \dots, p_d (see Kocis and Whiten [5]).

3 Faure sequence

This is a d -dimensional sequence.

The Faure sequence is a permutation of the Halton sequence, but it uses the same base r for each dimension. We choose r as the smallest odd prime integer such that $r \geq d$.

Note that the k -th dimension of a d -dimensional Faure sequence is different from the k -th dimension of a d' -dimensional Faure sequence as soon as the base r is different.

With usual notations, a_i are the coefficients of the r -adic decomposition of n

$$n = \sum_{i=0}^{R(n)} a_i r^i$$

We consider the following transformation T :

$$T : x = \sum_{k=0}^{R(n)} \frac{a_k}{r^{k+1}} \mapsto T(x) = \sum_{k=0}^{R(n)} \frac{b_k}{r^{k+1}}$$

with $b_k = \sum_{i=k}^{R(n)} C_i^k a_i \pmod{r}$ and C_i^k denote binomial coefficients.

The coefficients b_k are a permutation of the a_k .

Precision ... and reference ?????

The *Faure sequence* is defined by using successive transformations T^k :

$$\xi_n = (\varphi_r(n), T(\varphi_r(n)), \dots, T^{d-1}(\varphi_r(n)))$$

where φ_r is the Van der Corput sequence in base r .

The discrepancy of the sequence satisfies :

$$D_n^*(\xi) \leq C^d \frac{\log^d(n)}{n}$$

where C^d is a constant dependent on d and r : $C = \frac{1}{d!} \left(\frac{r-1}{2 \log r} \right)^d$.

The constant C^d tends to 0 with dimension.

The Faure sequence exhibits cycles of length r but cycles are not composed of increasing terms, except for the first dimension. For the same dimension, the Faure sequence has generally a smaller base than the Halton one, thus cycles are smaller too. Because we use the smallest prime number greater than the dimension d and not the d -th prime number.

Click there to reach the implemented part: [implementation](#).

4 Generalized Faure sequence

This is a d -dimensional sequence. Let r be the smallest odd prime integer, such that $r \geq d$.

The digit expansion of n in base r is given by $n = \sum_{i=0}^{R(n)} a_i(n)r^i$.

The *Generalized Faure sequence* is defined by :

$$\xi_n = \left(\sum_{k=0}^{R(n)} \frac{\xi_{n,k}^{(1)}}{r^{k+1}}, \dots, \sum_{k=0}^{R(n)} \frac{\xi_{n,k}^{(d)}}{r^{k+1}} \right)$$

with

$$\xi_{n,k}^{(j)} = \sum_{s=0}^{R(n)} c_{k,s}^{(j)} a_s(n), \quad j \leq d, k \leq R(n)$$

$c^{(j)} = (c_{k,s}^{(j)})_{0 \leq k \leq R(n), 0 \leq s \leq R(n)}$ and $c^{(j)} = A^{(j)} P^{j-1}$ where $A^{(j)}$ is a lower triangular invertible matrix such that $(a_{i,l}) \in \mathbb{F}_r$ and $P = (C_s^k)$ for $k \leq R(n), s \leq R(n)$ is built with the binomial coefficients.

The discrepancy of the sequence satisfies:

$$D_n^*(\xi) \leq C(d, r) \frac{\log^d(n)}{n}$$

where $C(d, r) \approx \frac{1}{d!} \left(\frac{r}{2 \log r} \right)^d$.

Click there to reach the implemented part: [implementation](#).

5 Nets and (t,s)-sequences

(t, s) -sequences are a group of sequences with a very regular distribution behaviour. Their points are placed into certain equally sized volumes of the unit cube for sequences of a fixed length. Chapter 4 of Niederreiter [7] well

describes theoretical aspects for such sequences. We just summarize in this section some definitions and properties of those sequences.

Definitions

- An *elementary interval* $E \in I^d$ is defined as $E = \prod_{i=1}^d [a_i b^{-d_i}, (a_i + 1)b^{-d_i}]$ where $a_i, d_i > 0$ are integers satisfying $0 \leq a_i \leq b^{d_i}$ for $1 \leq i \leq d$.
- Let $0 \leq t \leq m$ be integers. A (t, m, s) -net in base b is a point set P of b^m points in I^s such that the number of points in E is equal to b^t for every elementary interval E in base b with $\Pi(E) = b^{t-m}$.
- Let $t \geq 0$ be an integer. A sequence x_0, x_1, \dots of points in I^s is a (t, s) -sequence in base b if, for all integers $k \geq 0$ and $m > t$, the point set constituting of the x_n with $kb^m \leq n \leq (k+1)b^m$ is a (t, m, s) -net in base b .

Properties:

- Any (t, m, s) -net in base b is also a (u, m, s) -net in base b for integers $t \leq u \leq m$.
The same property holds for (t, s) -sequences.
Then smaller values of t mean stronger regularity properties.
- The discrepancy of a (t, m, s) -net P in base b with $m > 0$ satisfies:

$$ND_N(P) \leq B(s, b)b^t(\log N)^{s-1} + O(b^t(\log N)^{s-2})$$

where

$$B(s, b) = \begin{cases} \left(\frac{b-1}{2 \log b}\right)^{s-1} & \text{if either } s = 2 \text{ or } b = 2, s = 3, 4 \\ \frac{1}{(s-1)!} \left(\frac{\lfloor b/2 \rfloor}{\log b}\right)^{s-1} & \text{otherwise} \end{cases}$$

- The discrepancy of the first N terms of a (t, s) -sequence P in base b satisfies:

$$ND_N(P) \leq C(s, b)b^t(\log N)^s + O(b^t(\log N)^{s-1})$$

where

$$C(s, b) = \begin{cases} \frac{1}{s} \left(\frac{b-1}{2 \log b}\right)^s & \text{if either } s = 2 \text{ or } b = 2, s = 3, 4 \\ \frac{1}{s!} \frac{b-1}{2 \lfloor b/2 \rfloor} \left(\frac{\lfloor b/2 \rfloor}{\log b}\right)^s & \text{otherwise} \end{cases}$$

- For $m \geq 2$, a $(0, m, s)$ -net in base b can only exist if $s \leq b+1$.
A $(0, s)$ -sequence in base b can only exist if $s \leq b$.

Examples:

- The Van der Corput sequence is a $(0, 1)$ sequence in base b . In fact, if we consider the b^m points x_n with $kb^m \leq n < (k+1)b^m$ ($k \geq 0, m \geq 1$), every b -adic interval $[ab^{-m}, (a+1)b^{-m}]$ contains exactly one point x_n .
- The s -dimensional Sobol sequence is a (τ, s) -sequence in base 2, where $\tau = \sum_{i=1}^s \deg(P_i) - s$. It is called a LP_τ -sequence. Sobol sequence is described in the next point.
- The s -dimensional Faure sequence in base r is a $(0, s)$ -sequence where r is the smallest prime integer greater or equal than s .

6 Sobol sequence

The Sobol sequence is a d -dimensional sequence in base 2 and it is a (τ, d) -sequence. It is one of the most used sequences for Quasi-Monte Carlo simulation. It was first developed by Sobol [3] and it has been proved to have some additional uniformity property under some initialization conditions (see [9]). Its construction is based on primitive polynomials in the field \mathbb{Z}_2 and XOR operations.

Each dimension is a permutation of the Halton sequence with base 2 whenever $N = 2^d$. These permutations are generated from irreducible polynomials in \mathbb{Z}_2 . But they allow for certain correlations to develop, then they can produce regions where no points fall until N becomes very large.

The *Sobol sequence* is defined by:

$$\xi_n = \left(a_0 V_0^{(1)} \oplus \cdots \oplus a_{R(n)} V_{R(n)}^{(1)}; \dots; a_0 V_0^{(d)} \oplus \cdots \oplus a_{R(n)} V_{R(n)}^{(d)} \right)$$

where the $V_i^{(j)}$ are direction numbers (expressed as binary fraction) obtained from d different primitive polynomials and a_i denote the coefficients of the digit expansion of n in base $b = 2$, given by: $n = \sum_{i=0}^{R(n)} a_i 2^i$.

\oplus represents the bitwise exclusive OR operator (XOR). For explanation about XOR operation or primitive polynomials, we refer the reader to the Numerical Recipes in C [10].

To implement this sequence, we use an other expression for ξ_n depending only on the previous point and one direction number. This principle is detailed in the implemented part and is due to Antonov and Saleev [11].

The discrepancy of the sequence satisfies:

$$D_n^*(\xi) \leq C_d \frac{(\log n)^d}{n} + O\left(\frac{(\log n)^{d+1}}{n}\right)$$

where $C_d = \frac{2^{t(d)}}{d!(\log 2)^d}$ grows superexponentially with dimension, and for $K > 0$, $K \frac{d \log d}{\log \log d} \leq t(d) \leq \frac{d \log d}{\log 2} + O(d \log \log d)$. $t(d)$ grows superlinearly with dimension.

• **Definition of the constants V :**

- For each $j \leq d$ we first choose a primitive polynomial $P(j)$ with degree $s(j)$:

$$P(j) = x^{s(j)} + b_1 x^{s(j)-1} + \dots + b_{s(j)-1} x + 1$$

and we select $s(j)$ odd integers $c_i^{(j)}$ such that

$$c_i^{(j)} < 2^{i+1}, \quad 0 \leq i < s(j)$$

The choice for constants $c_i^{(j)}$ is not a easy step. Sobol' article ????? gives some explanations about this problem.

- Once we have chosen $P(j)$ and the $c_i^{(j)}$ for $i < s(j)$, we use the coefficients b_i through the recurrence relation :

$$c_i^{(j)} = 2b_1 c_{i-1}^{(j)} \oplus 2^2 b_2 c_{i-2}^{(j)} \oplus 2^{s(j)-1} b_{s(j)-1} c_{i-s(j)}^{(j)} \oplus 2^{s(j)} c_{i-s(j)}^{(j)} \oplus c_{i-s(j)}^{(j)}$$

to determine the $c_i^{(j)}$ for $i \geq s(j)$.

- Finally we calculate V by:

$$V_i^{(j)} = \frac{c_i^{(j)}}{2^{i+1}}$$

• **Uniformity property:** An additional uniformity property of the sequence is called by Sobol the *property A*.

- We define a *binary segment* of length 2^s as a set of points P_i whose subscripts satisfy the inequality $l2^s \leq i < (l+1)2^s$ where $l = 0, 1, \dots$.

We divide up the s -dimensional unit cube I^s by the planes $x_k = \frac{1}{2}$ into 2^s multidimensional small cubes, which represent binary parallelepipeds.

- **Property A:** If in any binary segment of length 2^s of the sequence P_0, \dots, P_i, \dots ,

all the points belong to different small cubes, then we say that the sequence satisfies property A.

Sobol [9] proved a sufficient and necessary condition on the direction numbers so that the property A is verified. A table of good numerical values for V is given for a dimension $s \leq 16$.

- **Property A'**: The property A can be extended to the property A' defined as follows.

We divide up the s -dimensional unit cube I^s by the planes $x_k = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ into 2^{2s} multidimensional small cubes. If in any binary segment of the sequence P_0, \dots, P_i, \dots of length 2^{2s} , all the points belong to different small cubes, then we say that the sequence possesses the property A'.

- Remark about the link between property A or A' and the dimension s : Note that the property A (resp. A') holds for subsequences of length 2^s (resp. 2^{2s}). In practice if s increases, it becomes difficult to verify the condition because we need to simulate at least 2^s (2^{2s}) points.

Click there to reach the implemented part: [implementation](#).

7 Niederreiter sequence

The *Niederreiter sequence* is a s -dimensional (t, s) -sequence in base b whose theoretical aspects are described in Niederreiter [7]. It is defined as:

$$\xi_n = \left(\sum_{j=0}^{R(n)} \frac{y_{n,j}^{(1)}}{b^{j+1}}, \dots, \sum_{j=0}^{R(n)} \frac{y_{n,j}^{(s)}}{b^{j+1}} \right)$$

with $n = \sum_{r=0}^{R(n)} a_r(n) b^r$ and

$$y_{n,j}^{(i)} = \sum_{r=0}^{R(n)} c_{j,r}^{(i)} a_r(n) \in \mathbb{F}_b$$

$C^{(i)} = (c_{j,r}^{(i)})$ is called the generator matrix of the i -th coordinate. An algorithm to compute the values is given in Niederreiter [7]. Initialization of the $(c_{j,r}^{(i)})$ is done at the beginning of the simulation.

The discrepancy of the sequence satisfies:

$$D_n^*(\xi) = O\left(\frac{(\log n)^s}{n}\right)$$

Construction of the $c_{jr}^{(i)}$: (in the next version)

The method is based on the formal Laurent series.

Remark: If b is a prime power and s an arbitrary dimension such that $s \leq b$, we can choose P_1, \dots, P_s as the linear polynomials $P_i(x) = x - b_i$ where b_1, \dots, b_s are distinct elements of F_b . Then the Niederreiter sequence is a $(0, s)$ -sequence in base b and we have for $1 \leq i \leq s$ and $j \geq 1$:

$$\begin{aligned} c_{jr}^{(i)} &= 0 \text{ if } 0 \leq r < j - 1 \\ c_{jr}^{(i)} &= (r/j - 1)b_i^{r-j+1} \text{ if } r \geq j - 1. \end{aligned}$$

Click there to reach the implemented part: [implementation](#).

8 General remarks on low discrepancy sequences

- Quasi-random numbers combine the advantage of a random sequence that points can be added incrementally, with the advantage of a lattice that there is no clumping of points.
- For large dimension s , the theoretical bound $(\log N)^s/N$ may only be meaningful for extremely large values of N . The bound in Koksma-Hlawka inequality gives no relevant information until a very large number of points is used.

Low discrepancy sequences are very useful for low dimension. In high dimension s , a lattice can only be refined by increasing the number of points by a factor 2^s .

- Orthogonal projections: if a d -dimensional sequence is uniformly distributed in I^d , then two-dimensional sequences formed by pairing coordinates should also be uniformly distributed. The appearance of non-uniformity in these projections is an indication of potential problems in using a quasi-random sequence for integration. This problem is developed in Morokoff and Caflish [6]. We will see that procedures like scrambling permutation can be suggested to improve the uniformity property while preserving the discrepancy.

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