

EFFICIENT COMPUTATION OF SOBOL' QUASI-RANDOM GENERATOR

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Abstract

Purpose of the study: The quasi-Monte Carlo method is an essential tool for modeling and analyzing various complex problems in engineering, physical sciences, finance, and business. The crucial element of the method is a sequence of deterministic quasi-random values, which is often obtained by using the Sobol' quasi-random generator. The purpose of this study is to consider the time complexity of generating the Sobol' sequence.

Methodology: Algorithms for determining the Sobol' sequence have been studied. The algorithms have been implemented in the Python programming language.

Main Findings: It is established that this sequence can be generated in the linear time provided that generated numbers are based on 32-bit or 64-bit integers. The main result of the paper is the algorithm, which enables this time-bound.

Applications of this study: The study can be applied in engineering, physical sciences, finance, and business.

Novelty/Originality of this study: It is shown that Sobol' sequence can be generated in linear time.

Keywords: *algorithm; time complexity; quasi-random generator; Sobol' sequence; quasi-Monte Carlo simulation*

INTRODUCTION AND LITERATURE REVIEW

Some crucial applications in engineering, physical sciences, finance, and business, to name just a few, are heavily dependent on Monte Carlo simulation ([Hammerley, 1964](#)), which is often one of the few available tools in econometrics ([Lyu, 2002](#)). The Monte Carlo methods are a broad class of statistical sampling techniques employed to provide numerical results of various challenging problems. In particular, Monte Carlo methods are ideal for establishing numerical solutions of very high-dimensional integrals, which can be applied, for example, to model complex financial instruments.

Standard Monte Carlo methods compute integrals of functions by using a set of points selected randomly. Since this approach admits various deficiencies, see, for example ([Morokoff, 1995](#)), a variation of this paradigm, called the quasi-Monte Carlo method had been proposed in the Fifties (see [Niederreiter, 1992](#) for the details). This method is a nonrandom variation of the Monte Carlo simulation, where randomly selected points are replaced with deterministic quasi-random values. Some interesting examples of quasi-random generators are the Halton sequence ([Halton, 1964](#)), the Faure sequence (as a particular instance of the Halton sequence), and recently introduced quasi-random based on generative neural networks ([Hofert, 2019](#)). However, the most prominent and frequently applied example of a quasi-random generator is the Sobol' sequence ([Sobol, 1967](#)).

The Sobol' sequence has been intensively investigated. Regarding the time complexity of the method, a more efficient Graycode implementation has been proposed ([Antonov, 1979](#)), while examples of some other aspects can be found in ([Joe 2003](#)) and ([Joe 2008](#)). Several implementations of the Sobol' sequence in various programming languages are also available, see for example ([Joe, 2019](#)).

METHODOLOGY

To obtain Sobol' sequence, we need to take a primitive polynomial of some degree s where the coefficients of the polynomial denoted by a_i are from the set $\{0,1\}$:

$$x^s + a_1x^{s-1} + a_2x^{s-2} + \dots + a_{s-1}x^1 + 1.$$

Loosely speaking, a primitive polynomial is a polynomial that cannot be resolved into factors. As an example, there are exactly two primitive polynomials of degree at most two: $x + 1$ and $x^2 + x + 1$.

The selected primitive polynomial is used to obtain the sequence of positive integers m_1, m_2, m_3, \dots as follows. The beginning of the sequence m_1, m_2, \dots, m_s can be chosen by a user so that the condition $m_i < 2^i$ is fulfilled for every $1 \leq i \leq s$. The rest of the sequence is for $i > s$ provided by the formula:

$$m_i = 2a_1m_{i-1} \oplus 2^2a_2m_{i-2} \oplus \dots \oplus 2^{s-1}a_{s-1}m_{i-s+1} \oplus 2^sm_{i-s} \oplus m_{i-s}.$$

In the above formula, \oplus denotes the bitwise exclusive operator. The obtained numbers are the basis for the sequence of real numbers v_1, v_2, v_3, \dots which are given by the formula:

$$v_i = \frac{m_i}{2^i}.$$



Finally, for $i \geq 1$, the point x_i of Sobol' sequence is obtained by

$$x = i_1 v_1 \oplus i_2 v_2 \oplus \dots$$

Here, i_k denotes the k -th bit from the right in the binary representation of i .

Note that the above definition leads to a straightforward but relatively inefficient implementation that provides the Sobol' sequence for a desired number of points. A more efficient implementation of this sequence is obtained by using the Gray code as follows.

Let z_i denote the index of the first bit 0 from the right in the binary representation of i . We can now obtain the sequence recursively by the following definition:

$$x_0 = 0 \text{ and } x_i = x_{i-1} \oplus v_{z_{i-1}} \text{ for } i \geq 1.$$

Note that with the Gray code approach, the same set of points is obtained as with the standard one, yet the points are different.

FINDINGS / RESULTS

We first present the Algorithm 1 called Zeros, which computes the sequence z_1, z_2, \dots, z_n , where z_i is the index of the first bit 0 from the right in the binary representation of i . The i -th iteration of the for loop of the algorithm calculates the wanted value for the integer i such the value of i is halved in every iteration of the inner while loop.

Algorithm 1: Zeros

Input: integer n

Output: sequence z_1, z_2, \dots, z_n , where z_i is the index of the first bit 0 from the right in the binary representation of i

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for  $i := 1$  to  $n$  do begin
     $t := 1$ ;
     $j := i$ ;
    while  $j \bmod 2 = 1$  do begin
         $j := \lfloor j/2 \rfloor$ ;
         $t := t + 1$ ;
    end;
     $z_i := t$ ;
end;

```

The sequence z_1, z_2, \dots, z_n obtained in the algorithm Zeros can be applied to compute the same number of points of Sobol' sequence as can be seen in Algorithm 2 called Sobol. The algorithm follows the definition of Sobol' sequence by using the Gray code as presented in the previous section. In order to enable the computation of a bitwise exclusive operator \oplus , it is provided that its operands are always integers. For this reason, the division with a power of two is postponed to the last loop of the algorithm. Note that the explicit computation of the sequence v_1, v_2, \dots, v_n is therefore not needed in the algorithm. This follows by the fact that the value of v_i is simply the value of m_i divided by 2.

Algorithm 2: Sobol

Input: polynomial a of degree s , number of points n

Output: Sobol' sequence x_0, x_1, \dots, x_n

```

Zeros( $n, z$ );
for  $i := 1$  to  $s$  do  $m_i := 2^i - 1$ ; // Determine  $m_1, m_2, m_3, \dots, m_s$  such that  $m_i < 2^i$ 
 $l := \lceil \log_2 n \rceil$ ;
for  $i := s+1$  to  $l$  do begin
     $m := m_{i-s} \oplus (m_{i-s} \cdot 2^s)$ ;
    for  $j := 1$  to  $s-1$  do
        if  $a_j \neq 0$  then
             $m := m_i \oplus (m_{i-j} \cdot 2^j)$ ;
end;
 $x_0 := 0$ ;
for  $i := 1$  to  $n$  do
     $x := x_{i-1} \oplus m_{z_i}$ ;
end;
for  $i := 1$  to  $n$  do
     $x_i := \frac{x_i}{2^l}$ ;

```

end;

It is next shown that the time complexity of computing Sobol' sequence depends on the running time of the algorithm Zeros. Let consider first the complexity of Zeros. Obviously, the number of iterations of the (inner) while $\log_2 n$ bounds loop. Since other statements of the body of the (outer) for loop can be executed in constant time and since the number of iterations of this loop equals n , the complexity of this algorithm is $(n \log n)$.

To provide the time complexity of the other parts of the algorithm Sobol, note first that the computation of the bitwise exclusive or operator \oplus can be done in constant time in most programming languages provided that the operands are 32-bit or 64-bit integers. Moreover, by using a bitwise arithmetic shift, the computation of a power of 2 can also be done in constant time. Since this also holds for multiplications and divisions, the time complexity of all loops except the second one is linear. In the second loop, the number of iterations of its inner loop equals $s - 1$. Since the value of s is constant, the time complexity of the second loop is also linear.

By the above discussion, we could conclude that the algorithm Zeros is the obstacle for the linear time complexity of the algorithm Sobol. Thus, a more efficient approach is suggested in the following two algorithms.

The algorithm gives the needed result ZerosP, where the sequence z_0, z_1, \dots, z_n is computed for $n = 2^k$. This algorithm is based on the observation, that for $1 \leq i \leq 2^k$ we have the following formula which can be easily confirmed by mathematical induction:

$$z_{i+2^k} = \begin{cases} z + 1, & z_i = k \\ z_i, & \text{otherwise} \end{cases}$$

Note that since $z_1 = 2$ and $z_2 = 1$, the above formula leads to Algorithm 3 called ZeroP.

Algorithm 3: ZerosP

Input: integer k

Output: sequence z_1, z_2, \dots, z_{2^k} , where z_i is the index of the first bit 0 from the right in the binary representation of i

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if  $k \leq 1$  then begin
     $z_1 = 2;$ 
     $z_2 = 1;$ 
end
else begin
    ZerosP( $k - 1$ );
    for  $i := 1$  to  $2^{k-1}$  do
        if  $z_i = k$  then  $z_{i+2^{k-1}} := z_i + 1$ 
        else  $z_{i+2^{k-1}} := z_i;$ 
end;
  
```

Since n need not be equal to a power of 2 in general, we need a procedure to establish the rest of the required values. The procedure is given in Algorithm 4.

Algorithm 4: FastZeros

Input: integer n

Output: sequence z_1, z_2, \dots, z_n , where z_i is the index of the first bit 0 from the right in the binary representation of i

```

 $k := \lceil \log_2 n \rceil;$ 
ZerosP( $k$ );
for  $i := 1$  to  $n - 2^k$  do
    if  $z_i = k + 1$  then  $z_{i+2^k} := z_i + 1$  else  $z_{i+2^k} := z_i;$ 
  
```

To see that the time complexity of FastZeros is linear, we first consider the running time of ZerosP. Note that the algorithm ZerosP computes z_1, z_2, \dots, z_{2^k} , where $2^k \leq n < 2^{k+1}$. Since the loop of ZerosP(i) contains 2^{i-1} steps and since ZeroP is called for every $1 \leq i \leq k$, the total number of steps of the algorithm can be bounded by

$$\sum_{i=1}^k 2^{i-1} = 2^k - 1.$$

Besides the call of ZerosP, which is performed in $2^k - 1$ and the computation of k , FastZeros contains the loop which computes the remaining entries $z_{2^k}, z_{2^k+1}, \dots, z_n$. Since this procedure is linear in the number of entries, the time complexity of FastZeros is bounded by (n) .

Note that from the above discussion, it follows that if FastZeros replace the call Zeros in Algorithm 2, the overall time complexity of the algorithm Sobol is linear.

DISCUSSION / ANALYSIS

All algorithms of the previous section have been implemented in the Python programming language. The algorithm Sobol has been tested for $n = 10^5, 10^6, 10^7, 10^8$. The results of computations are given in Table 1.

Table 1: Running times (s)

n	10^5	10^6	10^7	10^8
Sobol with Zeros	0.126	1.245	12.734	127.769
Sobol with FastZeros	0.091	0.905	9.029	95.948

Source: program in Python experiments

The results show that the version of Sobol with FastZeros outperforms the variant which uses the algorithm Zeros and confirms the time complexity analysis of the algorithms.

CONCLUSION

The Sobol' quasi-random generator is one of the most important means of generating quasi-random numbers that are involved in the quasi-Monte Carlo simulation. This simulation offers the numerical solution of very high-dimensional integrals required for solving difficult problems in science, engineering, finance, and business.

It is shown that the Sobol' sequence can be generated in linear time with respect to the number of points of the sequence. The presented algorithms are implemented in Python programming language, and their running times are tested for various points.

LIMITATION AND STUDY FORWARD

The obtained time complexity of the presented algorithm can be achieved only if all applied basic operations (a bitwise arithmetic shift, exclusive or operator, division, and multiplication) are performed in constant time in the corresponding computer program. Though this is the case for most of the programming languages and computers provided that the operands are 32-bit integers, this sometimes needs not to be true (in rare cases) when 64-bit integers are required. Note, however, that 64-bit integers are needed if the number of points of the sequence exceeds $2^{32} = 4294967296$.

Note also that the proposed method for fast computation of Sobol' sequence depends on recursion. Notwithstanding, since almost all modern imperative programming languages support recursion, this is not a severe limitation of the algorithm. It is true however, that programming languages are generally slower with recursion. Therefore, it would be interesting to devise a non-recursive version of the algorithm proposed in this work.

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