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A NUMERICAL STUDY ON HAMMERSLEY SEQUENCE AND FIBONACCI BASED LATTICE RULE FOR COMPUTATION OF MULTIDIMENSIONAL INTEGRALS

Venelin Todorov[1], Ivan Dimov[1], Valerij Dzurov[2],Tosho Stanchev[2], Ilian Tsvetkov[2], Valentin Dimitrov[2]

[1] DEPARTMENT OF PARALLEL ALGORITHMS, IICT, BULGARIAN ACADEMY OF SCIENCES
E-mail: venelin@parallel.bas.bg, ivdimov@bas.bg,

[2] ROUSSE UNIVERSITY "ANGEL KANCHEV"
E-mail: vdzhurov@yahoo.com

ABSTRACT: *In this paper we make a numerical study between Hammersley quasi-random sequence and Fibonacci based lattice rule for computing multidimensional integrals. The two methods have not been compared before and both are recommended in case of smooth integrands. The two quasi-Monte Carlo approaches are completely different thus it is a question of interest which one of them outperforms the other. We consider a case study with smooth integrand functions of different dimensions. A comparison with Sobol sequence for a fixed computational time is given.*

KEYWORDS: *Quasi-Monte Carlo sequences, multidimensional integrals, Hammersley sequence, Fibonacci lattice rule, Sobol sequence, applications.*

Introduction

High dimensional integrals are usually solved with Monte Carlo algorithms and quasi-Monte Carlo algorithms. The crude Monte Carlo method has rate of convergence $O(N^{-1/2})$ which is independent of the dimension of the integral, and that is why Monte Carlo integration is the only practical method for many high-dimensional problems. Much of the efforts to improve Monte Carlo are in construction of variance reduction methods which speed up the computation or to use quasi-random sequences [4]. Quasi-Monte Carlo methods use deterministic sequences that have better uniform properties measured by discrepancy [12]. They are usually superior to the Monte Carlo method as they have a convergence rate of $((\log N)^S/N)$, where N is the number of

samples and s is the dimensionality of the problem under consideration.

A low-discrepancy sequence is a sequence with the property that for all values of N, its subsequence x_1, ..., x_N has a low discrepancy. The discrepancy of a sequence is low if the proportion of points in the sequence falling into an arbitrary set B is close to proportional to the measure of B, as would happen on average (but not for particular samples. Specific definitions of discrepancy differ regarding the choice of B (hypersheres, hypercubes, etc.) and how the discrepancy for every B is computed (usually normalized) and combined (usually by taking the worst value). Low-discrepancy sequences are also called quasi-random or sub-random sequences, due to their common use as a replacement of uniformly distributed random numbers [11]. The "quasi" modifier is used to denote more clearly that the values of a low-discrepancy sequence are neither random nor pseudorandom, but such sequences share some properties of random variables and in certain applications such as the quasi-Monte Carlo method their lower discrepancy is an important advantage.

A low discrepancy sequence, such as the Faure, Halton, Hammersley, Niederreiter or Sobol sequences, is ”less random” than a pseudorandom number sequence, but more useful for such tasks as approximation of integrals in higher. This is because low discrepancy sequences tend to sample space ”more uniformly” than random numbers. It is a question of interest to know which sequence outperforms the other [10].

Lattice rules are based on the use of deterministic sequences rather than random sequences. They are a special type of so-called low discrepancy sequences. It is known that as long as the integrand is sufficiently regular, lattice rules outperform the basic Monte Carlo method and most of the other types of low discrepancy sequences [1].

Quasi Monte Carlo algorithms for numerical integration

Because any distribution of random numbers can be mapped onto a uniform distribution, and subrandom numbers are mapped in the same way, this article only concerns generation of subrandom numbers on a multidimensional uniform distribution. There are constructions of sequences known such that for their discrepancy:

$$D_N^*(x_1, \ldots, x_N) \leq C\frac{(\ln N)^s}{N}.$$

Here C is a certain constant, depending on the sequence. These sequences are believed to have the best possible order of convergence.

The standard M-dimensional Hammersley sequence [6] based on a number of samples N is simply composed of a first component of successive fractions 0/N, 1/N, ..., N/N, paired with M-1 1-dimensional van der Corput sequences [19], using as bases the first M-1 primes. The van der Corput sequence generates a

sequence of points in [0,1] which never repeats. For positive index I, the elements of the van der Corput sequence are strictly between 0 and 1. In particular, the I-th element of the van der Corput sequence is computed by writing I in the base B (usually 2) and then reflecting its digits about the decimal point. Let $b_1,...,b_{s-1}$ be coprime positive integers greater than 1. For given s and N, the s-dimensional Hammersley set of size N is defined by [7]

$$x(n) = (g_{b_1}(n), \ldots, g_{b_{s-1}}(n), \frac{n}{N})$$

for n = 1, ..., N. Then the discrepancy of the set is obtained in [10]:

$$D_N^*(x(1), \ldots, x(N)) \leq C \frac{(\log N)^{s-1}}{N}$$

where C is a constant depending only on b_1, ..., b_{s-1}. The above estimation for the discrepancy of the Hammersley sequence means that this is a low discrepancy sequence. The parameters of the algorithm are input: the integer I, the index of the element of the sequence 0 <= I; integer M, the spatial dimension, 1 <= M <= 100 and integer N, the "base" for the first component 1 <= N. Output is real R(M), the element of the sequence with index I.

The monographs of Sloan and Kachoyan [15], Niederreiter [13], Hua and Wang [10], Wang and Hickernell [20] and Sloan and Joe [14] provide comprehensive expositions of the theory of integration lattices. We implemented a specific lattice rule and compared its performance with an implementation of Hammersley sequence over integrals of smooth functions.

Let n be an integer, and a =($a_1,...,a_s$) be an integer vector modulo n. A set of the form [19]

$$P_n = \left\{ \left\{ \frac{ak}{n} \right\} = \left(\left\{ \frac{a_1 k}{n} \right\}, \ldots, \left\{ \frac{a_s k}{n} \right\} \right) \mid k = 1, \ldots, n \right\}$$

is called a lattice point set, where {x} denotes the fractional part of x. The vector a is called a lattice point or generator of the set. As one can see, the formula for the lattice point set is simple to program. The difficulty lies in finding a good value of a, such that the points in the set are evenly spread over the unit cube. The choice of good generating vector, which leads to small errors, is not trivial [8]. Complicated methods from theory of numbers are widely used, for example Zaremba's index or error of the worst function. We consider the following generating vector based on generalized Fibonacii numbers of corresponding dimensionality:

$$a = (1, F_{l+1}^{(s)}, ..., F_{l+s-1}^{(s)})), \quad n_l = F_l^{(s)},$$

where

$$F_{l+s}^{(s)} = F_l^{(s)} + F_{l+1}^{(s)} + ... + F_{l+s-1}^{(s)}, l = 0, 1, \ldots$$

with initial conditions

$$F_0^{(s)} = F_1^{(s)} = \ldots = F_{s-2}^{(s)} = 0, F_{s-1}^{(s)} = 1,$$

for l=0,1,…

The discrepancy of the set obtained by using the vector described above is asymptotically estimated in [9].

The number of calculation required to obtain the generating vector is O(ln n_l). The generation of a new point requires constant number of operations, thus to obtain a lattice set of the described kind consisting of n_l points, O(ln n_l) number of operations are necessary. However the discrepancies of the lattice point sets obtained by these two methods have larger upper bounds than those obtained by Korobov's method [1].

In experiments in the next section we use the well known quasi-random sequence of Sobol which is given as reference. They were first introduced by the Russian mathematician Ilya M. Sobol in 1967 [15] and later described in [16]. We use an adaptation of the INSOBL and GOSOBL routines in ACM TOMS Algorithm 647 [3] and ACM TOMS Algorithm 659 [2]. The original code can only compute the "next" element of the sequence. The revised code allows the user to specify the index of the desired element [18].

Numerical example and results

We will test the performance of the Hammersley sequence (HAM) and a particular lattice rule with generating vector, based on the generalized Fibonacci numbers of the corresponding dimensionality (FIBO) on multidimensional integrals of smooth functions of different dimensions. A comparison with Sobol quasi-random sequence (SOBOL) for a preliminary given computational time will be given. We will be interested which of the methods gives lowest relative errors for 1 minute. We consider examples of 4, 10 and 25 dimensional integrals.

Example 1.

$$\int_{[0,1]^4} x_1 x_2^2 e^{x_1 x_2} \sin(x_3)\cos(x_4) \approx 0.1089748630.$$

Exampe 2.

$$\int_{[0,1]^{10}} \frac{4x_1 x_3^2 e^{2x_1 x_3}}{(1+x_2+x_4)^2} e^{x_5+\cdots+x_{10}} \approx 14.808435.$$

Example 3.

$$\int_{[0,1]^{25}} \frac{4x_1x_3^2e^{2x_1x_3}}{(1+x_2+x_4)^2} e^{x_5+\cdots+x_{20}} x_{21}\dots x_{25} \approx 103.808.$$

Table 1: The relative error for 4 dimensional integral

N	FIBO	Time,s	HAM	Time,s
100	1.39e-1	0.001	2.44e-2	0.01
1000	9.27e-3	0.01	4.91e-3	0.17
10000	7.90e-4	0.09	7.84e-4	1.61
100000	3.40e-4	1.10	7.17e-5	12.4
1000000	2.68e-5	5.79	1.66e-6	74.7

Table 2: The computational time for 4 dimensional integral

time in seconds	FIBO	SOBOL	HAM
0.1	9.27e-3	5.17e-3	2.44e-2
1	3.26e-4	5.37e-5	1.22e-3
10	7.21e-6	1.43e-5	9.18e-5
60	9.10e-8	2.68e-7	3.61e-6

Table 3: The relative error for 10 dimensional integral

N	FIBO	Time,s	HAM	Time,s
100	8.35e-1	0.001	2.30e-1	0.01
1000	1.47e-1	0.08	1.55e-2	0.25
10000	4.21e-2	0.12	2.34e-3	0.98
100000	1.02e-2	0.91	7.55e-4	12.08
1000000	1.08e-3	6.27	1.56e-5	124.6

Table 4: The computational time for 10 dimensional integral

time in seconds	FIBO	SOBOL	HAM
0.1	9.82e-2	1.06e-2	5.94e-2
1	4.58e-2	9.15e-2	1.24e-3
10	1.37e-2	9.93e-4	9.46e-4
60	1.28e-3	1.38e-4	6.65e-5

Table 5: The relative error for 25 dimensional integral

N	FIBO	Time,s	HAM	Time,s
1000	9.84e-1	0.03	4.49e-1	0.17
10000	7.10e-1	0.11	1.53e-1	2.27
100000	1.97e-1	0.81	1.65e-4	12.55
1000000	9.09e-2	6.40	9.16e-5	147.1

Table 6: The computational time for 25 dimensional integral

time in seconds	FIBO	SOBOL	HAM
0.1	7.10e-1	2.50e-1	4.22e-1
1	1.21e-1	1.09e-1	1.13e-1
10	8.86e-2	1.85e-2	2.43e-2
60	7.13e-2	9.21e-3	2.78e-3

In the Table 1,3 and 5 are presented the relative error for the 4,10 and 25 dimensional integrals with Fibonacci lattice sequence (FIBO) and Hammersley quasi-random sequence (HAM) for a fixed number of points. In table 2,4,6 are presented the relative errors for 4,10 and 25 dimensional integrals with Sobol quasi-random sequence (SOBOL), FIBO and HAM for a fixed computational time which is a measure of the computational complexity. Obviously FIBO has the lowest computational complexity and is the fastest algorithm, while HAM and SOBOL are slower, because they need an additional time for generating the corresponding low discrepancy sequences. As can been seen from the results for 4 dimensional integral, the low discrepancy sequence of Hammersley produces more rapid convergence, and lower errors, than the Fibonacci lattice sequence for a given number of realizations of the random variable-see Table 1, but for a fixed computational time- Fibonacci sequence gives better results- see Table 2. In Table 2 Fibonacci gives better results than Hammersley sequence for a fixed computational time and better results than Sobol sequence with increasing the preliminary given time. Therefore Fibbonaci lattice rule is the best choice for low dimensional integrals- for one minute it gives relative error of 9.10e-8 which is better than Sobol and Hammersley sequences. For the 10-dimensional integral Hammersley gives lower relative errors than the Fibonacci algorithm- see Table 3. For a preliminary given time in seconds Sobol and Hammersley gives better results than Fibonacci-see Table 4. It is interesting that for 1 minute Hammersley gives 6.65e-5, which is better than Sobol-1.38e-4 and far better than FIBO- 1.28e-3. This means that for mid and high dimensions Hammersley sequence gives more reliable results than FIBO and it

can be successfully compete with one of the best quasi-random sequences of Sobol. For 25- dimensional integral as expected FIBO produces the worst results, while Hammersley sequence is more appropriate for higher dimensions- see Table 5. For a fixed computational time Hammersley again gives lower relative errors than Sobol- for 1 minute Hammersley gives 2.78e-3 which is better than Sobol with 1 order and better than FIBO with 2 orders- see Table 6. For higher dimensions the errors can not be small. However, Hammersley and Sobol sequences gives sufficient accuracy.

Conclusion

In this paper we analyze the performance of different quasi-Monte Carlo methods for multidimensional integrals. The Hammersley quasi-random sequence is compared with the Sobol sequence and the results are very precise for the multidimensional integrals under consideration, which shows the strength of the presented algorithm for low, mid and high dimensions.

Stochastic methods under consideration are an efficient way to solve problems that are described with multidimensional integrals. For example, stochastic methods have been successfully applied for sensitivity studies of large air pollution model in [5]. Such multidimensional integrals of smooth functions can be used to describe problems in quantum mechanics for Wigner kernel evaluation; in computational finance for evaluation of option pricing; for quick choice of frequent range for objects with plasma cover; for determining the type of dynamic objects with low effective reflecting surface or for increasing the efficiency of radiolocation systems with application of artificial intelligence.

This is the first time a particular 1-rank lattice rule based on Fibonacci lattice sequence is compared with Hammersley quasi-random sequence. There are several papers from authors in which Fibonacci lattice sequences is compared with Sobol sequence for different multidimensional integrals. Numerical experiments in this paper shows that Fibonacci sequence is the best choice for lower dimensions, as it was previously established. It is well known that as long as the integrand is sufficiently regular Fibonacci lattice rule outperforms other low discrepancy sequences for lower dimensions because of its lowest computational complexity and higher accuracy.

It is interesting that Hammersley sequence gives better results than Sobol with increasing the dimensionality of the integral. In the case of mid and high dimensional integrals it can be seen that Hammersley sequence produces lower relative errors for a fixed computational time. Tables show that for dimensional integral Sobol sequence gives better results than Hammersley, but for 10 and 25 dimensional integrals Hammersley sequence produces lower relative errors than Sobol sequences. In the future a scrambled version of Sobol sequence will be

presented and a comparison with the Hammersley sequence will be given. It will be interesting to compare Hammersley sequence with Halton and Niederreiter sequences, but this will be an object of a future study.

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