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An Optimal Monte Carlo algorithm for a Class of Multidimensional Integrals

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***Abstract*—An optimal stochastic approach for multidimensional integrals of smooth functions. This is the first time this optimal stochastic approach has been compared with other stochastic approaches for mid and high dimensions. The purpose of the present study is to compare the optimal algorithm with the lattice rules based on the generalized Fibonacci numbers of the corresponding dimension and to discuss the advantages and disadvantages of each method.**

I. Introduction

The Monte Carlo method has proven to be very useful tool for numerical analysis, particularly when the number of dimension ranging from medium to large. Monte Carlo simulation and quasi-Monte Carlo methods are the prevailing methods used to solve multi-dimensional problems in different areas. Both methods do not suffer from the „curse of the dimensionality" [2] This is the first time to study optimal stochastic algorithms for computing multidimensional integrals of smooth functions. The optimal approach has been established by Atanasov and Dimov in [1] but there aren't any comparison with other stochastic approaches up to now.

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II. Description of the Optimal Monte Carlo algorithm

Most Monte Carlo methods improve achieves better convergence using the idea of dividing the area of integration [2]. In the case where, in addition to the idea of dividing the area $\Omega = U^s$ (but without the recursive element), the information on the smoothness of the subintegral function is used, an increase in the order of convergence is achieved. Our first known results in this area with probability density $p(\mathbf{x}) = 1$, and splitting the area into equal parts in all directions are obtained by Dupach ([4]).

Theorem 1: (Dupach, [4]). Let $g(\mathbf{x})$ and all its first-order partial derivatives $\frac{\partial g}{\partial x_k}$ are continuous in Ω and bounded, i.e. for all $1 \leq k \leq s$: $\left|\frac{\partial g}{\partial x_k}\right| \leq L$, and there exist constants $c_1, c_2 > 0$, for which are fulfilled the following conditions

$$p_j \leq \frac{c_1}{N}, \qquad j = 1, \ldots, N, \qquad d_j \leq \frac{c_2}{N^{1/s}},$$

where d_j is the diameter of the subdomain Ω_j, i.e. $d_j = \sup_{\mathbf{x}_1,\mathbf{x}_2\in\Omega_j} |\mathbf{x}_1 - \mathbf{x}_2|$. Then for the estimation of the variance we obtain $\overline{\theta}^*_N$ in the case of $M = N \;\; N_j = 1, j = 1, \ldots, M$ and:

$$\mathbf{D}\overline{\theta}^*_N \leq c^2 L^2 N^{-1-2/s}, \quad \text{where} \quad c = sc_1c_2.$$

Using Chebyshev's inequality [**?**], [**?**], for the error $\overline{\theta}^*_N - I[g]$ we obtain

$$P\left\{|\overline{\theta}^*_N - I[g]| < \frac{c\ L}{\varepsilon}\ N^{-1/2-1/s}\right\} \geq 1 - \varepsilon^2, \qquad (1)$$

where ε is a small enough positive number.

Given the equation (1) it can be concluded that the probable error $\overline{\theta}^*_N - I[g]$ decreases in order $N^{-1/2-1/s}$, i.e. faster than $N^{-1/2}$. Obviously for large dimensions s the acceleration of the convergence order is relatively insignificant.

The same result for the order of convergence can be achieved in less favorable conditions, namely, only that the corresponding function is continuous. The proof is made by Dimov and Tonev ([3]), and the statement is formulated in the following theorem:

Theorem 2: (Dimov, Tonev; [3]). Let g is continuous in $\Omega \subset \mathbf{R}^s$ and there exist constants c_1, c_2, c_3, such that $p_j \leq c_1/N,\ d_j \leq c_2 N^{-1/s}$ and $S_j(\cdot, c_3) \subset \Omega_j,\ j = 1, \ldots, N$ (i.e. $M = N$ and $N_j = 1$), where $S_j(\cdot, c_3)$ is sphere with radius c_3. Then for the probable error r_N is fulfilled [2]:

$$r_N \leq 4\sqrt{2}\frac{c_1c_2}{c_3}\tau(g; d_{max})_{L_q}\ N^{-1/2-1/s},$$

where $d_{max} = \max_j d_j \;\; \tau(g;\delta)_{L_q}$ is the average modulus of continuity, that is,

$$\tau(g;\delta)_{L_q} = ||\omega(g,\cdot;\delta)||_{L_q} = \left(\int_\Omega (\omega(g,\mathbf{x};\delta))^q\ \mathrm{d}\mathbf{x}\right)^{1/q},$$

$$1 \leq q \leq \infty,\ \delta \in [0, d_{max}] \text{ and}$$

$$\omega(g,\mathbf{x};\delta) = \sup\{|\Delta_h\ g(\mathrm{t})| : \mathrm{t}, \mathrm{t}+h \in [\mathbf{x}-\delta/2, x+\delta/2]\cap\Omega\},$$

where Δ_h is the difference (forward) of the function g in the point t from first order, which in this case plays a role similar to the derivative but in a discrete sense.

Similar to the one obtained by Dupach, a higher order variance estimate can also be derived for a class of functions whose higher order derivatives are constrained by adding additional conditions for the choice of random points in the subdomains. Rayna Georgieva proves the following theorem [5]:

Theorem 3: Let we have domain $\Omega \in \mathbf{R}^s$ and the division of the domain $\Omega = \sum_{j=1}^M\ \Omega_j$, where every subdomain Ω_j is centrally symmetric with center p_j. Let $\xi^{(j)}$ is a random s-dimensional point, uniformly distributed in Ω_j, $\xi^{(j)'}$ is symmetric (about the center p_j) with $\xi^{(j)}$, i.e. $\xi^{(j)} + \xi^{(j)'} = 2\ p_j$. If the first and second partial derivatives of a function $g(\mathbf{x})$ are continuous in Ω and for all $k, l = 1, \ldots, s$ is fulfilled that

$$\frac{\partial^2 g}{\partial x_k\ \partial x_l} \leq L \qquad d_j = \sup_{x_1,x_2\in\Omega_j} |x_1 - x_2| \leq \frac{c_1}{N^{1/s}},$$

then $\mathbf{D}\ \overline{\theta}^{**}_N = c_2\ L^2\ N^{-1-4/s}$, where $\overline{\theta}^{**}_N = \sum_{j=1}^N \frac{V_j}{2}\ [g(\xi^{(j)}) + g(\xi^{(j)'})]$, V_j is the volume of the subdomain $\Omega_j \quad c = (0.5s^2c_1^{s+2})^2$.

There are various Monte Carlo approaches for numerical integration whose convergence order is $\mathcal{O}\left(N^{-\frac{1}{2}-\frac{k}{s}}\right)$. For $k = 1$ and $k = 2$ these methods can be constructed relatively easily [2], following Dupach's ideas for $k = 1$, described above (see the Theorem 1). But the situation changes when $k \geq 3$. Using the method of controlling the variance on interpolation polynomials, Atanasov and Dimov [1] formulate conditions for constructing a method with optimal order of convergence for s-dimensional functions from the class W^k. The optimal method requires $m * n^s$ points and is briefly described below [1].

For $n, s, k \geq 1$ we define integration formula of type Monte Carlo, depends on an integer parameter $m \geq 1$ and $\binom{s+k-1}{s}$ points in $[0,1]^s$ by the following way. Points $x^{(r)}$ are exactly a number of $\binom{s+k-1}{s}$ and they must fulfil the condition, that if for one polynom $P(x)$, so that for the degree of the polynom $\deg P \leq k$ is fulfilled $P(x^{(r)}) = 0$, then $P \equiv 0$. If $N = n^s$ for $n \geq 1$ we divide s dimensional hypercube $[0,1]^s$ into n^s *endless undercubes* K_j, i.e. $[0,1]^s = c_{i=1}^{n^s} K_j$ and $K_j = \prod_{i=1}^s [a_i^j, b_i^j)$, where $b_i^j - a_i^j = \frac{1}{n}$ for every $i = 1, \ldots, s$.. For every cube K_j we calculate the coordinates of $\binom{s+k-1}{s}$ points $y^{(r)}$, defined by $y_i^{(r)} = a_i^r + \frac{1}{n}x_i(r)$. We assume that we choose m random points $\xi_i(j,s) = (\xi_1(j,p), \ldots, \xi_s(j,p))$ from every cube K_j, such that all the points $\xi_i(j,p)$ are independent uniformly distributed random points, we calculate all $f(y^{(r)})$ and $f(\xi_i(j,p))$, and we calculate the Lagrange polynom of the function f in the point z using information about the functional values in the points $y^{(r)}$. We denote the polynom by $L_k(f,z)$. For every polynom P of max degree $k-1$ we have that $L_k(f,z) \equiv z$. Now we approximate

$$\int_{K_j} f(x)dx \approx \frac{1}{mn^s}\sum_{s=1}^m[(\xi(j,p)) - L_k(f,\xi(j,p))] + \int_{K_j} L_k(f,x)dx.$$

After that we sum for every $j = 1, \ldots, N$ and obtain:

$$I(f) \approx \frac{1}{mn^s}\sum_{j=1}^N\sum_{s=1}^m[(\xi(j,p)) - L_k(f,\xi(j,p))] + \sum_{j=1}^N\int_{K_j} L_k(f,x)dx.$$

$$\int_{K_j} f(x)dx \approx \frac{1}{mn^s}\sum_{s=1}^m[(\xi(j,p)) - L_k(f,\xi(j,p))] + \int_{K_j} L_k(f,x)dx.$$

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III. Numerical examples

We will test the optimal method on multidimensional integrals of smooth functions of different dimensions. We use the following notations: A==Adaptive stochastic approach, L=Latin Hypercube sampling, S=Sobol quasi-random sequence, F=Fibonacci lattice rule, O=optimal approach. For more information about the description of the different stochastic approaches, see [2], [6]. We must emphasise

Table I
RELATIVE ERROR FOR THE 3 DIMENSIONAL INTEGRAL DIMENSIONAL INTEGRAL

N	A	t	F	t	S	t	L	t	O	t
10^3	4.82e-3	0.17	1.21e-3	0.006	4.87e-4	0.47	6.14e-3	0.004	3.12e-5	0.81
10^4	1.07e-3	1.44	5.04e-4	0.07	1.56e-4	1.88	6.56e-4	0.06	2.05e-6	4.13
10^5	1.52e-4	10.9	5.34e-6	0.66	2.51e-5	15.6	1.34e-4	0.51	4.58e-7	31.62
10^6	5.11e-5	131	7.85e-7	7.02	7.43e-6	105.80	6.84e-5	5.22	6.72e-8	155
10^7	2.34e-5	1094	8.89e-8	79.7	1.58e-6	934	1.73e-5	17	5.34e-9	1053

Table II
RELATIVE ERROR FOR THE 3 DIMENSIONAL INTEGRAL

time(s)	C	A	F	S	L	O
1	1.05e-3	7.96e-3	2.34e-6	2.93e-4	5.11e-4	1.21e-5
5	6.84e-4	8.14e-4	8.47e-7	8.01e-5	7.32e-5	1.12e-6
10	4.79e-4	1.82e-4	4.89e-7	4.71e-5	4.32e-5	7.21e-7
100	1.57e-4	7.04e-5	6.53e-9	7.68e-6	5.32e-6	8.61e-8

Table III
RELATIVE ERROR FOR THE 4 DIMENSIONAL INTEGRAL

N	A	t	F	t	S	t	L	t	O	t
10^4	3.11e-4	1.97	2.61e-5	0.07	2.61e-5	2.14	5.29e-4	0.07	1.52e-5	4.81
10^5	2.44e-5	20.1	5.62e-6	0.99	5.93e-6	17.6	3.56e-4	0.60	7.96e-6	45.1
10^6	1.13e-5	210	5.86e-7	5.22	1.51e-6	193	4.36e-5	4.97	2.31e-7	352.6
10^7	8.11e-6	2035	8.38e-9	58	8.30e-7	1121	8.12e-6	47.1	8.16e-9	2651

Table IV
RELATIVE ERROR FOR THE 4 DIMENSIONAL INTEGRAL

time(s)	C	A	F	S	L	O
0.1	3.48e-3	3.59e-4	1.44e-5	4.07e-4	4.18e-4	4.22e-5
1	1.48e-3	2.85e-4	5.62e-6	3.54e-5	3.32e-4	2.31e-5
5	6.62e-4	9.18e-5	5.38e-7	5.26e-5	4.23e-5	1.12e-5
10	2.52e-4	1.36e-5	3.77e-7	6.50e-6	3.48e-5	7.53e-6
20	1.58e-4	2.08e-5	2.67e-8	4.55e-6	2.16e-5	6.54e-7

on the fact this is the first time a comprehensive experimental study with this optimal approach and other stochastic methods under consideration has been done.

Example 1. s=3.

$$\int\limits_{[0,1]^3} \exp(x_1x_2x_3) \approx 1.14649907. \quad (2)$$

Example 2. s= 4.

$$\int\limits_{[0,1]^4} x_1x_2^2e^{x_1x_2}\sin(x_3)\cos(x_4) \approx 0.1089748630. \quad (3)$$

Example 3. s= 5.

$$\int\limits_{[0,1]^5} \exp(-100x_1x_2x_3)(\sin(x_4)+\cos(x_5)) \approx 0.1854297367. \quad (4)$$

Example 4. s= 7.

$$\int\limits_{[0,1]^7} e^{1-\sum\limits_{i=1}^{3} sin(\frac{\pi}{2}.x_i)}.arcsin(sin(1)+\frac{\sum\limits_{j=1}^{7} x_j}{200}) \approx 0.75151101. \quad (5)$$

Example 5. s= 15.

$$\int\limits_{[0,1]^{15}} (\sum_{i=1}^{10} x_i^2)(x_{11}-x_{12}^2-x_{13}^3-x_{14}^4-x_{15}^5)^2 \approx 1.96440666. \quad (6)$$

Example 6. s= 25.

$$\int\limits_{[0,1]^25} \frac{4x_1x_3^2e^{2x_1x_3}}{(1+x_2+x_4)^2}e^{x_5+\cdots+x_{20}}x_{21}\ldots x_{25} \approx 108.808. \quad (7)$$

Example 7. s= 30.

$$\int\limits_{[0,1]^30} \frac{4x_1x_3^2e^{2x_1x_3}}{(1+x_2+x_4)^2}e^{x_5+\cdots+x_{20}}x_{21}\ldots x_{30} \approx 3.244540. \quad (8)$$

For smooth integrands without computational peculiarities Fibonacci lattice algorithm gives better results for lower dimensions, but it requires more random points when the dimensionality increases. The MC algorithm based on Latin hypercube sampling has higher accuracy for this case study with increasing the dimensionality of the integral. The adaptive MC algorithm is slower, but it requires smaller number of random points to achieve better accuracy even for higher dimensions. The efficiency of the optimal C algorithm is clearly seen for lower dimensions.

As the dimension increases, the computational time of the optimal method decrease due to the increased computational time of the Lagrangian interpolation polynomial. But for very high dimensions 25 and 30 the relative error for a fixed computational time is better than this achieved by the other stochastic methods. From the Tables it is obvious that for small dimensions the FIBO and Optimal method achieves the best accuracy for a fixed preliminary given time - see Tables II,IV,VI. For dimensions up to 10, the FIBO and Optimal methods achieve the smallest relative error for a given number of samples - see Tables I,III,V. The Optimal method is with 1 order better than the FIBO method for a fixxed number of samples, but the advantage of FIBO method is the significantly lower computational time. It is seen that for dimensions 10 and 15, the Optimal method gives relative errors for a fixed number of samples with at least 1

Table V
RELATIVE ERROR FOR THE 5 DIMENSIONAL INTEGRAL

N	A	t	F	t	S	t	L	t	O	t
10^3	2.15e-3	0.27	1.75e-4	0.007	5.29e-4	0.03	9.38e-3	0.007	2.75e-5	2.1
10^4	2.01e-3	2.43	1.28e-5	0.06	1.43e-4	0.3	3.44e-3	0.07	7.22e-6	2.3
10^5	6.91e-4	22.2	9.50e-6	0.61	2.36e-5	2.77	2.01e-3	0.69	2.36e-6	6.2
10^6	2.92e-4	219.5	5.47e-7	5.98	6.07e-6	24.2	1.80e-4	6.17	5.46e-7	20.0
10^7	8.21e-5	2043	8.71e-9	58.4	2.30e-6	245	2.46e-5	60.5	7.01e-8	105.1

Table VI
RELATIVE ERROR FOR THE 5 DIMENSIONAL INTEGRAL

time(s)	A	F	S	L	O
0.1	3.16e-3	3.48e-3	1.09e-5	1.34e-4	3.21e-3
1	1.08e-3	2.08e-3	5.58e-6	7.21e-5	8.54e-4
5	8.79e-4	8.20e-4	8.71e-7	1.54e-5	3.25e-4
10	5.85e-4	7.51e-4	4.15e-7	9.32e-6	8.65e-5
20	3.99e-4	6.95e-4	8.37e-8	7.39e-6	5.02e-5

Table VII
RELATIVE ERROR FOR THE 7 DIMENSIONAL INTEGRAL

N	A	t	F	t	S	t	L	t	O	t
10^4	1.07e-3	2.07	2.19e-3	0.11	2.27e-4	0.76	1.79e-3	0.13	2.13e-4	10.2
10^5	7.51e-4	19.3	6.19e-4	0.99	1.22e-4	7.45	2.53e-4	1.15	4.41e-5	40.2
10^6	6.30e-5	194	1.99e-5	9.81	4.71e-5	72.3	8.27e-5	10.32	1.27e-6	167.1
10^7	2.34e-5	1861	4.89e-7	94.2	9.45e-6	697	1.69e-5	101.2	1.45e-7	595.1

Table VIII
RELATIVE ERROR FOR THE 7 DIMENSIONAL INTEGRAL

time(s)	A	F	S	L	O
0.1	2.38e-2	3.11e-2	2.38e-3	1.85e-3	2.37e-3
1	8.87e-3	2.88e-3	6.19e-4	1.85e-4	3.37e-4
5	5.16e-3	3.76e-3	8.81e-5	9.79e-5	1.38e-4
10	1.28e-3	6.71e-4	1.88e-5	8.36e-5	8.78e-5
20	2.03e-3	4.28e-4	3.87e-6	5.46e-5	6.87e-5

Table IX
RELATIVE ERROR FOR THE 15 DIMENSIONAL INTEGRAL

N	A	t	F	t	S	t	L	t	O	t
10^3	3.16e-3	9.24	5.34e-2	0.08	2.04e-3	0.98	1.06e-2	0.12	7.54e-3	27.4
10^4	1.49e-3	88	1.22e-3	0.93	2.89e-4	9.3	7.33e-3	1.07	6.51e-4	81.5
10^5	5.76e-4	847	3.08e-4	9.65	1.13e-4	93.8	1.54e-3	10.11	7.29e-5	242.1
10^6	1.29e-4	8235	1.37e-5	96.9	1.93e-5	935	1.14e-4	99.6	8.29e-6	720.2

order better than FIBO and Sobol, see Tables VII and IX, with FIBO

Table X
RELATIVE ERROR FOR THE 15 DIMENSIONAL INTEGRAL

time(s)	A	F	S	L	O
1	9.96e-1	6.30e-3	1.10e-3	3.64e-3	3.51e-2
5	7.72e-2	1.68e-3	2.45e-4	7.32e-4	1.23e-2
10	1.33e-2	5.89e-3	9.48e-5	1.94e-4	9.63e-3
20	3.03e-2	1.66e-3	9.87e-6	4.05e-5	7.51e-3
100	8.11e-3	5.04e-4	8.17e-7	4.03e-6	9.51e-5

Table XI
RELATIVE ERROR FOR THE 25 DIMENSIONAL INTEGRAL

N	O	t,s	S	t,s	L	t,s
10^3	3.77e-3	2.03	1.47e-1	0.4	7.54e-1	0.02
10^4	3.18e-3	19.52	5.68e-2	5.64	5.39e-2	0.15
10^5	5.33e-5	181	7.21e-3	33.4	2.11e-2	1.07
10^63	3.11e-5	1234	2.89e-3	161	1.71e-4	8.21

Table XII
RELATIVE ERROR FOR THE 25 DIMENSIONAL INTEGRAL

time,sec	O	S	L
1	7.24e-2	9.51e-2	2.11e-2
5	8.16e-3	5.76e-2	1.61e-2
10	5.18e-3	2.71e-2	9.58e-3
20	3.13e-3	8.28e-3	7.87e-3

Table XIII
RELATIVE ERROR FOR 30 DIMENSIONAL INTEGRAL

N	O	t,s	S	t,s	L	t,s
10^3	2.01e-2	5.4	1.18e-1	0.42	8.81e-1	0.02
10^4	6.53e-3	14.5	8.40e-2	4.5	6.19e-2	0.14
10^5	1.35e-3	145	1.18e-2	30.2	2.78e-2	1.16
10^6	2.11e-4	1290	9.20e-3	168	9.86e-3	8.61

Table XIV
RELATIVE ERROR FOR 30 DIMENSIONAL INTEGRAL

time,sec	O	S	L
1	4.38e-1	1.01e-1	2.38e-2
5	1.16e-2	7.76e-2	1.81e-2
10	8.11e-3	5.71e-2	9.48e-3
20	4.63e-3	1.28e-2	7.87e-3

achieving better accuracy in much less time - see Tables VIII and X. The adaptive algorithm is suitable for higher dimensions because of the small number of samples to achieve the preliminary given relative error. The Adaptive algorithm performs better than FIBO and Sobol - see Tables XI and XIII. Analyzes show that for high 25 and 30 samples, the Optimal MC approach outperforms LHS and Sobol's quasi-Monte Carlo algorithm - see Tables XII and XIV, where the LHS method produce better results than the Sobol QMC approach. Here we do not test Adaptive approach, because of the significant amount of time and FIBO method which gives unreliable relative errors for the high dimensional case.

IV. CONCLUSIONS

The efficiency of the optimal Monte Carlo algorithm for the calculation of multidimensional integrals has been presented. The optimal approach appears to be an efficient stochastic solution to solve this kind of problem, because we demonstrate here its reliability for calculating integrals with smooth integrands in a relatively small subregion of the original integration domain regardless of the dimension.

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