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An Optimized Monte Carlo Approach for Multidimensional Integrals Related to Intelligent Systems

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***Abstract*—We study an optimized Monte Carlo algorithm for solving multidimensional integrals related to intelligent systems. Recently Shaowei Lin consider the difficult task of evaluating multidimensional integrals with very high dimensions which are important to machine learning for intelligent systems. Lin multidimensional integrals with 3 to 30 dimensions, related to applications in machine learning, will be evaluated with the presented optimized Monte Carlo algorithm and some advantages of the method will be analyzed.**

I. Introduction

TEN YEARS ago Shaowei Lin in his works [4], [5] consider the important problem of evaluating multidimensional integrals used in intelligent systems. The first multidimensional Lin integrals are of the form

$$\int_\Omega p_1^{u_1}(x)\dots p_s^{u_s}(x)dx, \tag{1}$$

and the second Lin integrals are of the form

$$\int_\Omega e^{-Nf(x)}\phi(x)dx, \tag{2}$$

where $f(x)$ and $\phi(x)$ are multidimensional polynomials with an integer N. Up to now multidimensional Lin integrals (1) and (2) are computed unsatisfactory with deterministic [10] and algebraic methods [9], and it is known that the Monte Carlo (MC) methods [3], [7], [8] outperforms the deterministic methods which suffer from the so called „curse of dimensionality" [3] especially for higher dimensions.

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The paper is organised as follows. The description of the optimal stochastic approach is given in Section II. The numerical study with Lin multidimensional integrals is given in Section III. Finally some concluding remarks are given in Section IV.

II. The optimal stochastic approach

We adapt the idea of the original MC method developed by Atanassov and Dimov twenty years ago [1].

Let d and k be integers, $d, k \geq 1$. We consider the class

$$F_0 \equiv \mathbf{W}^k(\|f\|; U^d) \tag{3}$$

(sometimes abbreviated to $\mathbf{W}^k$) of real functions f defined over the unit cube $U^d = [0,1)^d$, possessing all the partial derivatives

$$\frac{\partial^r f(\mathbf{x})}{\partial x_1^{\alpha_1}\dots\partial x_d^{\alpha_d}},\ \ \alpha_1+\dots+\alpha_d = r \leq k, \tag{4}$$

which are continuous when $r < k$ and bounded in sup norm when $r = k$. The semi-norm $\|\cdot\|$ on $\mathbf{W}^k$ is defined as

$$\|f\| = \sup\left\{\left|\frac{\partial^k f(\mathbf{x})}{\partial x_1^{\alpha_1}\dots\partial x_d^{\alpha_d}}\right|,\ \ \alpha_1+\dots+\alpha_d = k,\ \mathbf{x}\equiv(x_1,\dots,x_d)\in U^d\right\}. \tag{5}$$

Now for $n, s, k \geq 1$ we construct a MC integration formula depending on $m \geq 1$ and $\binom{s+k-1}{s}$ points in $[0,1]^s$. Points $x^{(r)}$ are exactly $\binom{s+k-1}{s}$ and if for $P(x)$ 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 $[0,1]^s$ into n^s *endless undercubes* K_j, i.e.

$$[0,1]^s = c_{i=1}^{n^s} K_j$$

and

$$K_j = \prod_{i=1}^{s}[a_i^j, b_i^j),$$

$$b_i^j - a_i^j = \frac{1}{n},$$

$i = 1, \ldots, s$. For every cube K_j we evaluate the coordinates of $\binom{s+k-1}{s}$ points $y^{(r)}$, determined by

$$y_i^{(r)} = a_i^r + \frac{1}{n} x_i^{(r)}.$$

We choose m random points $\xi_i(j,s) = (\xi_1(j,p), \ldots, \xi_s(j,p))$ from every cube K_j, so all $\xi_i(j,p)$ are independent uniformly distributed random points, and calculate $f(y^{(r)})$ and $f(\xi_i(j,p))$, and the Lagrange polynom of f in z to obtain $L_k(f,z)$.. Now for every P of max degree $k-1$ we have $L_k(f,z) \equiv z$. For every $j = 1, \ldots, N$ we sum and obtain:

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

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

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

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

Thus an optimal MC approximation with an optimal order of convergence $\mathcal{O}\left(N^{-\frac{1}{2}-\frac{k}{d}}\right)$ for d-dimensional functions from the class W^k is derived.

III. Numerical results

We will use the following notations: LHSM=Latin Hypercube sampling *method* [6], SOBOLS=Sobol quasi-random *sequence* [2], OPTIMAL=*optimal* approach under consideration. In the Tables below the relative errors (RELERR) obtained with the three approaches are given for the corresponding multidimensional integral (MI).

We study the following Lin multidimensional integrals (1) and (2): Example 1. s=3.

$$\int_{[0,1]^3} \exp(x_1 x_2 x_3) \approx 1.14649907. \tag{6}$$

Example 2. s= 4.

$$\int_{[0,1]^4} x_1 x_2^2 e^{x_1 x_2} \sin(x_3) \cos(x_4) \approx 0.1089748630. \tag{7}$$

Example 3. s= 5.

$$\int_{[0,1]^5} \exp(-100 x_1 x_2 x_3)(\sin(x_4) + \cos(x_5)) \approx 0.1854297367. \tag{8}$$

Example 4. s= 7.

$$\int_{[0,1]^7} e^{1-\sum_{i=1}^{3} sin(\frac{\pi}{2}.x_i)} .arcsin(sin(1) + \frac{\sum_{j=1}^{7} x_j}{200}) \approx 0.75151101. \tag{9}$$

Example 5. s= 15.

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

Example 6. s= 25.

$$\int_{[0,1]^{25}} \frac{4x_1 x_3^2 e^{2x_1 x_3}}{(1+x_2+x_4)^2} e^{x_5+\cdots+x_{20}} x_{21} \ldots x_{25} \approx 108.808. \tag{11}$$

Example 7. s= 30.

$$\int_{[0,1]^{30}} \frac{4x_1 x_3^2 e^{2x_1 x_3}}{(1+x_2+x_4)^2} e^{x_5+\cdots+x_{20}} x_{21} \ldots x_{30} \approx 3.244540. \tag{12}$$

Table I
RELERR for the 3-MI.

N	SOBQMC	t	LHSM	t	OPTMC	t
10^3	4.87e-4	0.47	6.14e-3	0.004	3.12e-5	0.81
10^4	1.56e-4	1.88	6.56e-4	0.06	2.05e-6	4.13
10^5	2.51e-5	15.6	1.34e-4	0.51	4.58e-7	31.62
10^6	7.43e-6	105.80	6.84e-5	5.22	6.72e-8	155
10^7	1.58e-6	934	1.73e-5	17	5.34e-9	1053

Table II
RELERR for the 3-MI for a fixed time.

time(s)	SOBOLS	LHSM	OPTIMAL
1	2.93e-4	5.11e-4	1.21e-5
5	8.01e-5	7.32e-5	1.12e-6
10	4.71e-5	4.32e-5	7.21e-7
100	7.68e-6	5.32e-6	8.61e-8

Table III
RELERR for the 4-MI.

N	SOBOLS	t,s	LHSM	t,s	OPTIMAL	t,s
10^4	2.61e-5	2.14	5.29e-4	0.07	1.52e-5	4.81
10^5	5.93e-6	17.6	3.56e-4	0.60	7.96e-6	45.1
10^6	1.51e-6	193	4.36e-5	4.97	2.31e-7	352.6
10^7	8.30e-7	1121	8.12e-6	47.1	8.16e-9	2651

For the 3-dimensional integrals for a number of samples $N = 10^7$ the best approach is OPTIMAL - it gives a relative error $5.34e-9$ -see Table I and for a preliminary given time in seconds the best approach for 100s is OPTIMAL- the relative error is $8.61e-8$ in Table II. For the 4-dimensional integrals for a number of samples $N = 10^7$ the best approach is OPTIMAL - it gives a relative error $8.16e-9$ -see Table III and for a preliminary given time in seconds the best approach for 20s is OPTIMAL- the relative error is $6.54e-7$

Table IV
RELERR FOR THE 4-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
0.1	4.07e-4	4.18e-4	4.22e-5
1	3.54e-5	3.32e-4	2.31e-5
5	5.26e-5	4.23e-5	1.12e-5
10	6.50e-6	3.48e-5	7.53e-6
20	4.55e-6	2.16e-5	6.54e-7

Table V
RELERR FOR THE 5-MI.

N	SOBOLS	t,s	LHSM	t,s	OPTIMAL	t,s
10^3	5.29e-4	0.03	9.38e-3	0.007	2.75e-5	2.1
10^4	1.43e-4	0.3	3.44e-3	0.07	7.22e-6	2.3
10^5	2.36e-5	2.77	2.01e-3	0.69	2.36e-6	6.2
10^6	6.07e-6	24.2	1.80e-4	6.17	5.46e-7	20.0
10^7	2.30e-6	245	2.46e-5	60.5	7.01e-8	105.1

Table VI
RELERR FOR THE 5-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
0.1	1.34e-4	3.21e-3	1.09e-4
1	7.21e-5	8.54e-4	5.58e-5
5	1.54e-5	3.25e-4	1.71e-6
10	9.32e-6	8.65e-5	8.15e-7
20	7.39e-6	5.02e-5	5.46e-7

Table VII
RELERR FOR THE 7-MI.

N	SOBOLS	t,s	LHSM	t,s	OPTIMAL	t,s
10^4	2.27e-4	0.76	1.79e-3	0.13	2.13e-4	10.2
10^5	1.22e-4	7.45	2.53e-4	1.15	4.41e-5	40.2
10^6	4.71e-5	72.3	8.27e-5	10.32	1.27e-6	167.1
10^7	9.45e-6	697	1.69e-5	101.2	1.45e-7	595.1

Table VIII
RELERR FOR THE 7-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
0.1	2.38e-3	1.85e-3	2.37e-3
1	6.19e-4	1.85e-4	3.37e-4
5	8.81e-5	9.79e-5	1.38e-4
10	1.88e-5	8.36e-5	8.78e-5
20	3.87e-6	5.46e-5	6.87e-5

in Table IV. For the 5-dimensional integrals for a number of samples $N = 10^7$ the best approach is again OPTIMAL - it gives a relative error $7.01e-8$ -see Table V and for a preliminary given time in seconds the best approach for 20s is again the optimal approach - the RELERR is $8.37e-8$ in Table VI. For the 7-dimensional integrals for a number of samples $N = 10^7$ the best approach is again OPTIMAL -

Table IX
RELERR FOR THE 15-MI.

N	SOBOLS	t,s	LHSM	t,s	OPTIMAL	t,s
10^3	2.04e-3	0.98	1.06e-2	0.12	7.54e-3	27.4
10^4	2.89e-4	9.3	7.33e-3	1.07	6.51e-4	81.5
10^5	1.13e-4	93.8	1.54e-3	10.11	7.29e-5	242.1
10^6	1.93e-5	935	1.14e-4	99.6	8.29e-6	720.2

Table X
RELERR FOR THE 15-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
1	1.10e-3	3.64e-3	3.51e-2
5	2.45e-4	7.32e-4	1.23e-2
10	9.48e-5	1.94e-4	9.63e-3
20	9.87e-6	4.05e-5	7.51e-3
100	8.17e-7	4.03e-6	9.51e-5

Table XI
RELERR FOR THE 25-MI.

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

Table XII
RELERR FOR THE 25-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
1	9.51e-2	2.11e-2	7.24e-2
5	5.76e-2	1.61e-2	8.16e-3
10	2.71e-2	9.58e-3	5.18e-3
20	8.28e-3	7.87e-3	3.13e-3

Table XIII
RELERR FOR THE 30-MI.

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

Table XIV
RELERR FOR THE 30-MI FOR A FIXED TIME.

time,s	SOBOLS	LHSM	OPTIMAL
1	1.01e-1	2.38e-2	4.38e-1
5	7.76e-2	1.81e-2	1.16e-2
10	5.71e-2	9.48e-3	8.11e-3
20	1.28e-2	7.87e-3	4.63e-3

it gives a relative error $1.45e - 7$ -see Table VII and for a preliminary given time in seconds the best approach for 20s is now the Sobol approach SOBOLS - the relative error is $3.87e - 6$ in Table VIII. For the 15-dimensional integrals for a number of samples $N = 10^6$ the best approach is again OPTIMAL - it gives a relative error $8.29e - 6$ -see Table IX and for a preliminary given time in seconds the best approach for 100s is again the Sobol approach - the relative error is $8.17e - 7$ in Table X. For the 25-dimensional integrals for a number of samples $N = 10^6$ the best approach is again OPTIMAL - it gives a relative error $3.11e - 5$ -see Table XI and for a preliminary given time in seconds the best approach for 20s is now the optimal approach - the relative error is $3.13e - 3$ in Table XII. For the 30-dimensional integrals for a number of samples $N = 10^6$ the best approach is again OPTIMAL - it gives a relative error $2.11e - 4$ -see Table XIII and for a preliminary given time in seconds the best approach for 20s is the optimal approach - the relative error is $4.63e - 3$ in Table XIV. From all the results we can conclude that for a preliminary given number of samples the optimal approach OPTIMAL always outperforms the Sobol approach SOBOLS, but the optimal approach is a computationally expensive algorithm, and sometimes for a preliminary given time in seconds the Sobol approach SOBOLS or even the Latin hypercube sampling approach LHSM outperforms the optimal approach OPTIMAL.

IV. Conclusion

In this paper an optimal Monte Carlo approach for computing Lin multidimensional integrals (1) and (2) which are important for machine learning in intelligent systems has been presented. This is the first time a specific optimal approach is used for evaluating multidimensional integrals in intelligent systems and also the comparison between the three methods has never been performed before. In our case study the Sobol sequence, the Latin hypercube sampling algorithm and the optimal Monte Carlo approach have been compared on some important Lin multidimensional integrals. The optimal Monte Carlo is one of the best available algorithms for high dimensional integrals and one of the few possible methods, because the deterministic methods are impractical for higher dimensions. At the same time the optimal method is suitable to deal with 30-dimensional problems for less than a minute on a laptop. It is an important element since this may be crucial in some control test examples in intelligent systems. In the future the scope of our work will be develop other optimal Monte Carlo approaches based on other techniques.

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