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A NEW METHOD OF VARIANCE REDUCTION IN MONTE CARLO INTEGRATION

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ABSTRACT

The Monte Carlo technique can be used as a method of statistical trials to calculate surface areas or object volumes by employing random numbers. It is especially helpful for complicated functions or irregular shapes in higher dimensional spaces. In this work, relying on a multinomial distribution, we give a fresh new look on Hit-or-Miss integration and present a technique called Extended Monte Carlo Integration (EMCI) by expressing the integral area of univariate functions in different forms. By taking the average of estimates from these forms it is possible to increase efficiency while maintaining a reasonable calculation speed. The application of this technique is demonstrated by using single-variable functions in the unit square. The method can be generalized to higher dimensions. There are very common cases in physics, chemistry, medicine, genetics and biology where there is no explicit function defining the region or the volume to be estimated. In these cases, instead of various function expressions, different rotations and reflections of the figure or object can be used. A distinct advantage of our method is its applicability to these problems. Investigating the suitability of the method to multi-core processors also seems promising.

Keywords: Crude Monte Carlo, Efficiency, Hit-or-Miss integration, Monte Carlo, Monte Carlo integration, Random number generator, Variance reduction.

1. INTRODUCTION

The use of simulation techniques extends to all fields of science. Simulations using random numbers are called Monte Carlo methods. Many mathematical or applied problems can be solved by Monte Carlo techniques, which rely on the repetition of random trials. This approach is a widely used numerical method employing random numbers produced by computers.

The Monte Carlo method is not restricted to the generation of random processes. In some cases the estimation of certain constants such as the mean of a random variable, areas of surfaces or volumes of objects can be calculated by using random numbers. The integrations of complicated functions in two- or higher-dimensional spaces are other possible scenarios where Monte Carlo methods can be used. There are several methods of Monte Carlo integration, for example: Evans and Swartz (1999), Fishman (1996), Gentle (2005), and Lemieux (2009). The Crude Monte Carlo inserts the random number into the function and calculates the average of the values obtained. This popular method is preferred in practice since it is fast and efficient. On the other hand, Hit-or-Miss Monte Carlo casts n points into the space of function and finds the ratios of points by using an indicator function on the integration regions. In this approach the outcome of each point generation is either success (within the integration region) or failure (outside of the integration region). Therefore the outcome of an experiment with n random points will have a binomial distribution.

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Here we present a new Hit-or-Miss integration technique, called the Extended Monte Carlo Integration (EMCI) by defining several integration regions in a two-dimensional space. The resulting distribution will rely on a multinomial distribution and will increase the efficiency of the estimation. The generalization of the technique to higher dimensions is possible and is worth further investigation.

This paper is organized as follows: Section 1 is the introduction. In Section 2, we summarize the usage of Monte Carlo integration method and present the general principles of our technique. In Section 3, we calculate expected variance reductions on six different functions, namely sin(x), e^{-x}, $\sqrt{x}$, x^2, x^3, and $(27/4)x(1-x)^2$. Section 4 presents simulation results for these functions, which serve as demonstrations supporting our theoretical arguments. Section 5 compares the speed of our method with the conventional single-area usage. In Section 6, our method is compared with the Crude Monte Carlo technique. Application of EMCI to higher dimensions is discussed in Section 7. The last section presents general conclusions.

2. THE NEW METHOD FOR HIT-OR-MISS MONTE CARLO

In two-dimensional applications of Hit-or-Miss Monte Carlo with n random trials, if x points fall within the region A, the area of this sub-region can be estimated by

$$\hat{S}_A = \frac{x}{n} S \,. \qquad (1)$$

Here, S is the area of the regular-shaped region enveloping surface A. This approach is also used for the integration problems. Consider a single-variable function f to be integrated within the unit interval:

$$I = \int_0^1 f(x)dx. \qquad (2)$$

This integral can be estimated by considering the region between the x axis and the curve $f(x)$. The estimator must be unbiased and must have a small variance. Several variance reduction techniques have been developed to increase efficiency of the estimators. These are well documented in simulation literature: McGeoch (1992; L'Ecuyer (1994); Fishman (1996); Evans and Swartz (1999); Law and Kelton (2000); Gentle (2005); Ross (2006); Lemieux (2009). Here, we will introduce a new variance reduction method suitable for the Hit-or-Miss technique, on which there is not adequate work.

2.1 Usage of Several Curves Simultaneously

The integral region may occupy only a small portion of the rectangle and there is no reason to restrict it to its present position. We can define several curves leading to the same estimation value. Let f be a function within the unit square. We define a set with eight elements using a binary operation $\circ$ based on the following motions of the curve $f(x)$:

a) The curve $f(x)$ is not moved. This is the identity operation: Curve $f(x)$.
b) It is rotated 90°clockwise around the center of the square: Curve $f(1-y)$.
c) It is rotated 180°clockwise around the center of the square: Curve $1- f(1-x)$.
d) It is rotated 270°clockwise around the center of the square: Curve $1- f(y)$.
e) It is reflected in the vertical line $x = 1/2$. Curve $f(1-x)$.

f) It is reflected in the horizontal line $y = 1/2$. Curve $1- f(x)$.
g) The curve (c) is reflected in the line $y = 1-x$. Curve $1- f(1-y)$.
h) The curve (d) is reflected in the line $y = x$. Curve $f(y)$.

These eight positions under the binary operation form a closed group and the area under the curve $f(x)$ can be calculated by using the corresponding region in anyone of these eight elements of this set. Table 1 is the *multiplication table* for the group defined by ∘.

Table 1. The multiplication table for the group defined by ∘

	a	b	c	d	e	f	g	h
a	a	b	c	d	e	f	g	h
b	b	c	d	a	g	h	f	e
c	c	d	a	b	f	e	h	g
d	d	a	b	c	h	g	e	f
e	e	h	f	g	a	c	d	b
f	f	g	e	h	c	a	b	d
g	g	e	h	f	b	d	a	c
h	h	f	g	e	d	b	c	a

Example: The corresponding graphs are depicted in Figure 1 for the special case Beta curve $f(x) = 6.75x(1-x)^2$. In a, c, e, and f, the curve will be compared by the value of the random number obtained from the y generator. In other curves, the function value is obtained from y variable and comparison is made with x generator.

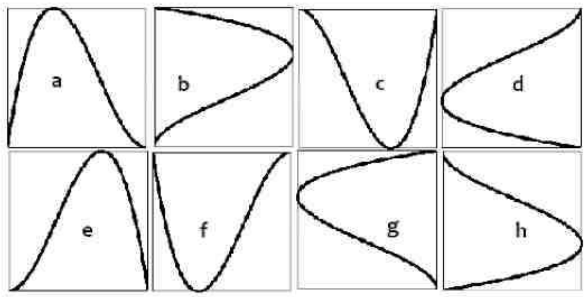

Figure 1. Eight possible representations for the $f(x) = 6.75x(1-x)^2$

When the point falls within the area under the curve the value of an indicator function is increased by 1 as shown below:

if (y ≤ f(x)) na=na+1.
if(x ≤ f(1-y)) nb=nb+1
if (y ≥ 1- f(1-x)) nc=nc+1
if (x ≥ 1- f(y)) nd=nd+1
if (y ≤ f(1-x)) ne=ne+1
if (y ≥ 1- f(x)) nf=nf+1

if ($x \geq 1-f(1-y)$) ng=ng+1
if ($x \leq f(y)$) nh=nh+1.

If a total of n points are cast within the unit square, one can use any of the counts na, nb, …, nh for estimating the area. But here it may be recommendable to use more than one indicator and then take the mean of the areas as the final estimator. We investigated the following possibilities:

1. Use only a single curve
2. Use the mean of the eight curves
3. Use the reflections of the curves using x as the range, a, c, e, and f.
4. Use the mean of the four rotations, a, b, c, and d.

The cases (2), (3), and (4) are depicted in Figure 2.

We simulated the above cases for determining the variance reductions and execution times. The data are summarized in Table 2. The variances are obtained from 1000 runs of the simulation each having 10000 point pairs. In order to determine the speeds, simulation is run for 100,000,000 points. As a measure of efficiency the ratio of variance reduction to the execution time can be used. By combining several curves the execution time increased, but considering the variance reduction this is a reasonable price for the efficiency obtained. According to the last column of Table 2, usage of a single curve is

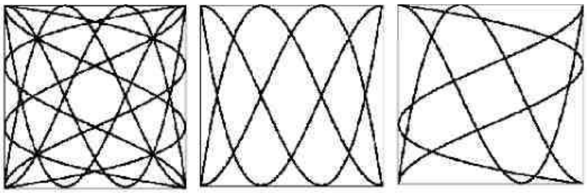

Figure 2. Some possible combinations for the $f(x) = 6.75x(1-x)^2$ curve

very inefficient. Case 2 gives highest efficiency followed by cases 4 and 3, but these last two have rather close values. Below we describe our method in detail for the reflections case.

Table 2. The variances and execution times of different applications in Beta function

	Variance	Variance Reduction (%)	Execution Time (Sec.)
Single Curve	$2.44\text{x}10^{-5}$	1.00	10.11
Eight Curves	$4.32\ \text{x}10^{-6}$	5.66	20.65
Four Rotations	$5.80\ \text{x}10^{-6}$	4.21	15.83
Four Reflections	$7.27\ \text{x}10^{-6}$	3.36	14.89

2.2 Reflections of f(x)

Reflections method is presented by Sezgin (2010) as an initial version of this study. The reflections with respect to x = 1/2 and y = 1/2 lines use the x variable as the domain. Here we define the following curves: Down1 = $f(x)$, Down2 = $f(1-x)$, Up1 = 1 - $f(x)$, and, Up2 = 1 - $f(1 - x)$. Here, Down2 is the reflection of Down1 in x = 1/2 vertical line. Up1 and Up2 are the horizontal reflections of Down1 and Down2 curves in line y = 1/2. This approach is partly similar to antithetic variables by the usage of 1-x. But there is an original contribution by the addition of horizontal reflections Up1 and Up2. Therefore, in functions of a single variable, instead of two estimators in antithetic variables we provide four estimators and use the sample space more efficiently. The situation is depicted in Figure 3 for the function $f(x) = x^2$. Let us denote the four integral estimates obtained from these regions as $\hat{I}_1$, $\hat{I}_2$, $\hat{I}_3$, and, $\hat{I}_4$. As an efficient estimation method we propose using the mean of these four estimates:

$$\hat{I} = \frac{\hat{I}_1 + \hat{I}_2 + \hat{I}_3 + \hat{I}_4}{4}. \qquad (3)$$

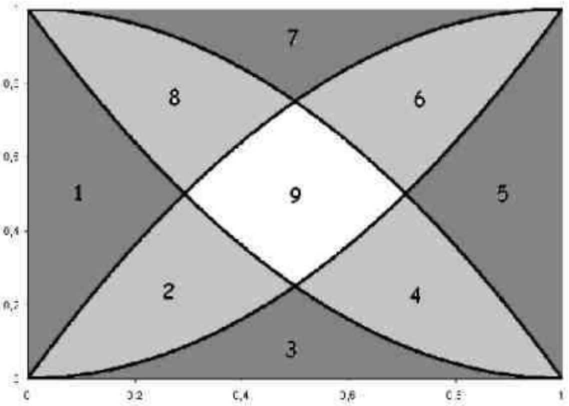

Figure 3. Joint usage of four regions for the integral of $f(x)= .x^2$ showing regions employed once (light shaded) and twice (dark shaded)

The four graphs define nine different sub-regions when they are superimposed. The integral estimate $\hat{I}$ contains data obtained from 8 mutually exclusive regions. Each of the regions 1, 3, 5, and 7 are added twice in forming $\hat{I}$. Regions 2, 4, 6 and 8 are added only once, whereas region 9 does not have any contribution. Therefore, in terms of sub-regions we can write

$$\hat{I} = \frac{2(x_1+x_3+x_5+x_7)+x_2+x_4+x_6+x_8}{4n} \qquad (4)$$

Let X_1, X_2, ⋯, X_9 be the random variables showing the number of points falling within the regions 1, 2, ⋯, 9 when n points are cast into the unit square. In a realization of the simulation experiment of size n with k mutually exclusive and collectively exhaustive regions these random variables will have

$$\sum x_i = n. \qquad (5)$$

X_i variables will have probabilities p_i satisfying

$$\sum p_i = 1. \qquad (6)$$

This situation defines the multinomial distribution for *X* values

$$P(x_1, x_2, ..., x_k) = \frac{n!}{x_1! x_2!, ..., x_k!} p_1^{x_1} p_2^{x_2} ... p_k^{x_k} . \qquad (7)$$

It is well known that the random variable X_i has mean $\mu_i = np_i$, and variance $\sigma_i^2 = np_i(1-p_i)$. The covariance between two variables is $\sigma_{ij} = -np_i\, p_j$. It is possible to calculate the mean and variance of the EMCI reflection estimate by using formulas related to a linear function of random variables $X_1, X_2, \cdots, X_k$. Let

$$Y = \sum a_i X_i . \qquad (8)$$

Then the mean and variance of *Y* are

$$E(Y) = \mu_Y = \sum_{i=1}^{k} a_i E(X_i) . \qquad (9)$$

$$Var(Y) = \sigma_Y^2 = \sum_{i=1}^{k} a_i^2 \sigma_i^2 + 2\sum_{i<j} a_i a_j \sigma_{ij} . \qquad (10)$$

The multinomial probabilities can be obtained by considering curves and axes around the sub-regions. For example, in $f(x) = x^2$ the area of the first sub-region will be:

$$p_1 = \int_0^{1-\sqrt{2}/2} \left\{(1-x)^2 - x^2\right\} dx = 0.1381 . \qquad (11)$$

$$p_2 = \int_0^{1-\sqrt{2}/2} \left\{1-(1-x)^2 - x^2\right\} dx + \int_{1-\sqrt{2}/2}^{1/2} \left\{(1-x)^2 - x^2\right\} dx = \frac{7-4\sqrt{2}}{12} = 0.1119 .$$

and

$$p_3 = \int_0^{1/2} x^2 dx + \int_{1/2}^{1} (1-x^2) dx = 0.0833 .$$

The symmetry of the curves will imply that $p_1 = p_5$, $p_2 = p_4 = p_6 = p_8$ and $p_3 = p_7$. By using these values it is possible to calculate the variance of $\hat{I}$ as $0.4412/(16n^2)$.

For $f(x) = x^2$ the performance of mean estimator against the single curve estimator is

$$\frac{\frac{Var(\hat{I}_1)}{Var(T)}}{(4n)^2} = \frac{2/(9n^2)}{0.4412/(16n^2)} = \frac{0.2222}{0.0276} = 8.06 . \qquad (12)$$

Therefore, the integral using only a single region has a variance eight times higher than our new method. In our application, one does not need to be concerned about sub-regions and their areas. Here, we presented them in a simple function to demonstrate the performance of our new method.

2.3 Rotations of f(x)

A curve $f1 = f(x)$ in the unit square may be rotated clockwise around the center of the square by 90 , 180 , and 270 degrees giving curves $f2$, $f3$, and $f4$ respectively. Since two random numbers are needed for a hit-or-miss integration, we use both generators as the domain for the function. The functions are defined as:

f1: $f(x)$
f2: $f(1-y)$
f3: $1- f(1-x)$
f4: $1- f(y)$.

From these curves $f1$ and $f3$ correspond to down1 and up2 curves of the reflection system. In the second and fourth cases the roles of x and y variables are interchanged. 1 is added to the indicator functions when $x< f(1- y)$ and $x> f(1-y)$, respectively. The performance of the rotations is discussed in the next section. For the Beta function studied above, it was slightly slower but more efficient than the reflection method. Since it requires the calculation of the function four times, it may be rather slow for very complicated functions.

3. VARIANCE REDUCTIONS FOR VARIOUS FUNCTIONS

We demonstrated above the performance of our method for the Beta function. In this section we calculate the outcomes of five more examples of integration for the reflection method:

1. Trigonometric function $\sin(x)$
2. Exponential function e^{-x}
3. Square root function $\sqrt{x}$
4. Square function x^2
5. Cubic function x^3

These functions partition the unit square into $k = 9$ regions. The multinomial probabilities for these sub-regions are presented in Table 3.

Table 3. The multinomial probabilities of nine sub-sections for the integration of five different functions

	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9
$Sin(x)$	0.175	0.040	0.245	0.040	0.175	0.040	0.245	0.040	0.001
e^{-x}	0.043	0.112	0.213	0.112	0.043	0.112	0.213	0.112	0.040
$\sqrt{x}$	0.083	0.112	0.138	0.112	0.083	0.112	0.138	0.112	0.109
x^2	0.138	0.112	0.083	0.112	0.138	0.112	0.083	0.112	0.109
x^3	0.095	0.123	0.031	0.123	0.095	0.123	0.031	0.123	0.253

Table 4. The coefficients for the sum of X_i variables in estimation of the total of four sub-regions

	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9
$Sin(x)$	2	1	2	1	2	1	2	1	0
e^{-x}	2	1	2	1	2	1	2	1	4
$\sqrt{x}$	2	3	2	3	2	3	2	3	4
x^2	2	1	2	1	2	1	2	1	0
x^3	2	1	2	1	2	1	2	1	0

In our estimator the sum of the points used in the calculation of $\hat{I}$ may be expressed in terms of X_i variables as a linear combination of these areas by $\sum a_i X_i$. The coefficients a_i are presented in Table 4. Here we observe that sin(x), x^2, and x^3 have the same coefficients. In the square root there are many intersections between regions; this reduces the efficiency. The coefficients in Table 4 and probabilities in Table 3 are used to determine the variance of our estimator as in Table 5 by employing equation (10). The last function in Table 5 represents the Beta function $f(x) = 12x(1 - x)^2$. We scaled it by changing the constant to 6.75 in order to equate the maximum of $f(x)$ to 1. That function partitions the unit square into 19 sub-regions.

Table 5. The variances of integral estimations for six different functions by using a single integral area and the average of four sub-sections

	Variances	Var(Reflection)	Ratio
$Sin(x)$	0.2479	0.0086	28.92
e^{-x}	0.2325	0.0206	11.31
$\sqrt{x}$	0.2222	0.0276	8.06
x^2	0.2222	0.0276	8.06
x^3	0.1875	0.0316	5.93
$6.75x(1-x)^2$	0.2461	0.0790	3.12

4. SIMULATION RESULTS

In order to test our theoretical arguments, we carried out Monte Carlo simulations to integrate the six aforementioned functions. For each function we used 1000 runs, each having n = 10000 random points cast into the unit square. The entries in Table 6 are obtained by dividing the average variance of sub-regions to the variance of the EMCI estimators. The findings strongly agree with our arguments presented in Section 3. The greatest variance reduction is obtained by using the average of the eight curves. In certain cases, such as sine and exponential functions, this reduces the variance more than twice of reflection and rotation alternatives. Reflection and rotation have comparable performances, although the latter is slightly better in Beta function. Reflection requires the calculation of the integrated function twice whereas eight curves and rotation methods require this calculation four times. Therefore the relative speeds must also be taken into account for preference among methods.

We also conducted series of simulations to assess the effect of sample size and compare the performances of various random number generators. For this purpose we used 25 different random number generators of various families. All these generators exhibit similar behaviors. Our proposed EMCI method approaches the true parameter value faster than any single integration region. In Figure 4, we present the errors of sin(x) integrals in reflection method for the Linear Congruential Generator with multiplier 48271 and modulus 2^{31} -1 as an example. The examination of this figure indicates that the Down1 and Up2 regions compensate the bias effects of each other. They move to opposite directions and balance each other. The same pattern is seen in Down2 and Up1 regions. Since these pairs are located on opposite corners, an increase in one of them implies a decrease in the other. This is the same situation we observed in multinomial random variables. Regions with large intersections have a positive correlation, as seen in Down1 and Down2 or Up1 and Up2 cases. The correlations of regions are presented in Table 7.

Table 6. The variance ratio comparisons of the average variance of single sub-regions with the variance of the EMCI estimates

	Eight Curves	Reflection	Rotation
$sin(x)$	55.7	25.0	27.0
e^{-x}	24.0	11.1	11.3
$\sqrt{x}$	9.3	8.1	8.0
x^2	9.3	8.0	8.1
x^3	6.8	5.6	5.8
$6.75x(1-x)^2$	5.7	3.4	4.2

Table 7. The correlations between integration regions for the sin(x) integral

	Down1	Down2	Up1
Down2	0.601280	1	
Up1	-0.67895	-0.85012	1
Up2	-0.94150	-0.66130	0.70334

Factors affecting the magnitude of the variance reduction are as follows:

1. The amount of unused area will increase the variance of the EMCI estimator. For example, the x^2 has a smaller unused region compared to x^3 and the improvement in this case is higher. Negative covariances due to sub-region 9 are not reflected in formula (10) for some functions because they have $a_9 = 0$.

2. Multiple usages of sub-regions will decrease the efficiency of EMCI because this situation will induce positive correlations between components. Consider, for example, two random variables of the form

$$T = X_1 + X_2 + X_3 + X_4 \tag{13}$$

and

$$S = 2X_1 + X_2 + X_3, \tag{14}$$

given that $p_1 = p_4$. In this case expected values of T and S are equal but the variance of S is larger than the variance of T. By formula (10) we get

$$\sigma_S^{\ 2} = \sigma_T^{\ 2} + 2np_1. \tag{15}$$

Therefore, a large intersection of areas will increase the variance of $\hat{I}$ and this will reduce the efficiency. In Tables 5 and 6 the worst situation is that of the Beta function because it has the largest intersection areas.

3. If all sub-regions are included at least once in the summation formula, the least usage frequency can be subtracted from all cells. It is obvious that if m is the minimum coefficient, then

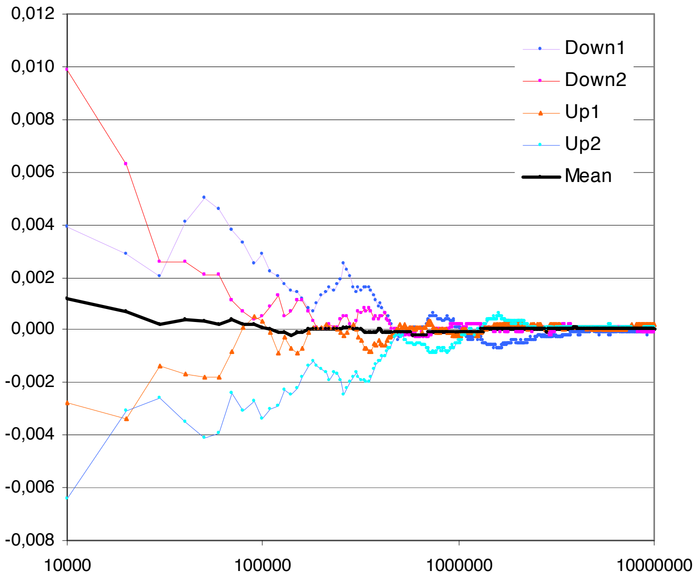

Figure 4. The error of Sin(x) integration for sample sizes from 10 thousand to 10 million

$$\sum mx_i = m\sum x_i = mn \tag{16}$$

is a constant and has zero variance. The only contribution to the estimator variance comes from cells having excess usages. For example, the smallest coefficient of the square root function is 2 and it can be subtracted from all coefficients, giving a_i values 0, 1, 0, 1, 0, 1, 0, 1, and 2. The same remark applies to e^{-x}. In $\sqrt{x}$ and e^{-x} sub-regions 2, 4, 6, and 8 have roughly the same size but the frequently used sub-region 9 is almost three times larger in $\sqrt{x}$. This decreases the efficiency of reflection estimator for the square root compared to the exponential.

These observations suggest the potential benefit of using rectangular areas other than the unit square. We can use a larger Y axis to minimize curve intersections. For example, in $\sqrt{x}$, the Y axis may have length $h = \sqrt{2}$ in order to eliminate the sub-region 9. There will be eight sub-regions with coefficients 2, 1, 2, 1, 2, 1, and 2. Subtracting regions with small coefficients, four very large portions will remain. This causes a great improvement in the estimation and reduces the variance 0.22222/0.01266 = 17.55 times. Increasing the rectangle height, h, will minimize the intersection but the unused area may also increase. Moreover, the variance of the EMCI will be multiplied by h^2. Therefore, increasing h may not be beneficial in some cases. For example, choosing h = 1.6875 in Beta distribution will eliminate several intersections, but the final estimator will have only an improvement of 2.56.

5. TIMINGS

We tested the running times of the single and EMCI programs by a simulation comprising of n = 100,000,000 points. Total time requirements (in seconds) are presented in Table 8. The concerned programs coded in Fortran Power Station 4.0 compiler were executed on an Intel Pentium 4, CPU 3.06 GHz processor with 2.00 GB of RAM on a Microsoft Windows XP Professional Version 2002 platform. The results show that our proposed method is rather fast. In several cases Eight Curves is almost as fast as the Rotation method. When the function is complex, such as sine, exponential and square root cases, the Reflection has a distinct advantage. The slowest function is the e^{-x} but still, it requires only 80% more time compared to the single integration in Reflection method. The extra time requirements can be considered negligible compared to the variance reductions provided by our estimator.

Table 8. Time (sec.) comparison for single and EMCI estimators for simulations with 100,000,000 points

Function	Single	Eight Curves	Reflection	Rotation	Eight/ Single	Reflection/ Single	Rotation/ Single
$\sin(x)$	32.0	102.3	56.3	102.2	3.2	1.8	3.2
e^{-x}	39.6	133.2	71.9	130.9	3.4	1.8	3.3
$\sqrt{x}$	25.6	82.3	45.8	79.5	3.2	1.8	3.1
x^2	10.0	17.1	14.0	14.0	1.7	1.4	1.4
x^3	9.6	16.8	13.4	13.8	1.8	1.4	1.4
$6.75x(1-x)^2$	10.1	20.7	14.9	15.8	2.0	1.5	1.6

6. COMPARISON WITH CRUDE MONTE CARLO

Evans and Swartz (1999) state that, “Discussion of the rejection algorithm brings up to the first integration technique in the text, sometimes referred to as Hit-or-Miss integration. However this method is mostly of historical interest.” In widely used Crude Monte Carlo method, the values of random numbers are directly inserted into the function to be integrated and the mean is calculated as

$$\hat{I}_c = \frac{1}{n}\sum_{i=1}^{n} f(x_i)\,. \tag{17}$$

Since $\hat{I}_c$ has a smaller variance compared to the Hit-or-Miss estimator $\hat{I}_h$, Monte Carlo integration sources recommend $\hat{I}_c$ in practice. This difference can be seen by comparing the variances. In the unit square, since $f(x) \leq 1$, the difference of variances is larger than zero as seen below:

$$\begin{aligned}\sigma_h^2 - \sigma_c^2 &= \frac{I}{n} - \frac{I^2}{n} - \frac{1}{n}E\{f^2(x)\} + \frac{I^2}{n} \\ &= \frac{I}{n} - \frac{1}{n}E\{f^2(x)\} = \frac{1}{n}\int_0^1 f(x)(1-f(x))dx.\end{aligned}$$

The usage of EMCI will improve the Hit-or-Miss technique as discussed in previous sections. According to our simulations, EMCI becomes very efficient and has a competitive advantage against the Crude estimator, as seen in Table 9. The Crude estimator will have a smaller variance only when it is used with a variance reduction technique such as the antithetic variable.

Table 9. Variances of Crude Monte Carlo and Reflection EMCI methods obtained from 1000 simulation runs, each having n=10000 points (Entries must be multiplied with 10^{-6})

Function	Crude	EMCI
$\sin(x)$	6.01	0.81
e^{-x}	6.01	0.81
$\sqrt{x}$	5.26	1.22
x^2	8.85	2.81
x^3	12.6	7.36
$6.75x(1-x)^2$	8.17	3.09

Our method has a distinct advantage in certain estimation problems:

- Crude Monte Carlo can be improved by the usage of antithetic variates but this method does not always work. For example, if the integrand is symmetric there is no gain. In this case EMCI reflection in y=1/2 can be beneficial. Consider the parabola $y=4x(1-x)$. The antithetic variable will give the same equation. But defining the second curve as $y=1-4x(1-x)$ will improve the estimation 1.8 times. A more effective application is to cut the upper curve in two parts as $y=(2x-(1+\sqrt{2}))^2$ and $y=(y-(1-\sqrt{2}))^2$ and replace them to the left and right of the integrand. This application may be called Cut and Paste EMCI. The rectangle of length $\sqrt{2}$ will extend from $(1-\sqrt{2})/2$ to $(1+\sqrt{2})/2$. This application reduces the variance of the estimate 8.2 times.

- In some situations the Crude Monte Carlo can not be used because there is no function representing the area or volume to be assessed. These cases involve two- or three-dimensional spaces and arise in many practical applications. The following studies can be mentioned as examples:

a) In multi-dimensional Nuclear Magnetic Resonance (NMR) experiments quantitative information can be obtained by peak volume integration as depicted in Figure 5. In this case the Hit-or-Miss technique is the most efficient way (Romano et al., 2008).

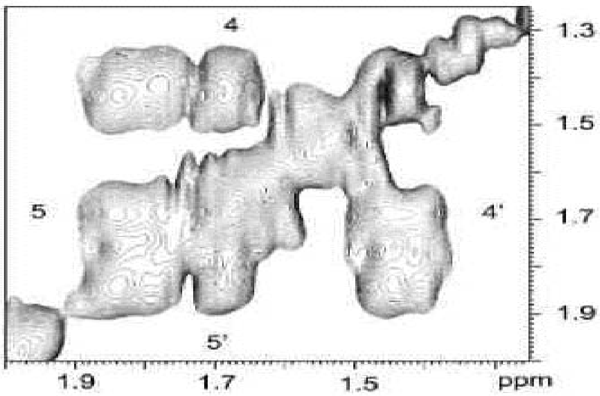

Figure 5. Nuclear magnetic resonance (NMR) spectra to be integrated

b) In order to assess the growth patterns of hepatocellular carcinoma with the aid of stochastic modeling, Saftoiu et al. (2004) use the Hit-or-Miss method for estimating the volume of tumors. According to their study this Monte Carlo technique gives more reliable results compared to the analysis of histological and ultrasonographic characteristics.

c) Hit-or-Miss Monte Carlo integration can be used to find virial coefficients of some volumes in Molecular Physics (Vlasov et al., 2002).

d) The Hit-or-Miss Monte Carlo method is used in path importance sampling and implementation for Markovian path simulations in atomistic modeling techniques (de Koning et al., 2005). Here, the purpose of predictive modeling and simulation at the atomistic level is to characterize and quantify the atomistic unit mechanisms that control the macroscopic behavior of complex systems. This objective is common to many fields of research, including chemistry, physics, biology, and materials science.

e) In some applications the location and even the shape of the area or volume to be inspected may be unknown (Naiman and Priebe (2001); Priebe et al. (2001). Therefore, in detecting a signal of unknown location and geometry in a Gaussian random field (GRF) and detecting a cluster of unknown location and geometry in a point process or a multinomial sequence there is no explicit function to be integrated. Examples of this application are multinomial sequences in molecular genetics, spatial point processes in digital mammography, and Gaussian random fields in PET scan brain imagery. Another application is the case of marked spatial Poisson processes applied to minefield reconnaissance using multiple scan geometries. Romano et al. (2008) prepared a toolbox called MatCAKE for integrating 2D NMR spectra in Matlab. It is possible to implement EMCI as a built-in software for some medical or physical equipment.

f) In studying cirrus clouds by remote-sensing Takano and Liou (1995) compute scattering, absorbtion and polarization properties of ice crystals with various irregular structures. In this study the incident photons are traced with a Hit-or-Miss Monte Carlo method.

7. APPLICATION TO HIGHER DIMENSIONS

The present work demonstrates the performance of the proposed technique for some simple univariate functions. It is worth studying the application for different volumes in higher dimensions. In reflection EMCI by introducing each variable as U_i or $1 - U_i$ in functions with d variables, it is possible to obtain 2^d different Down functions. By extending the calculations to the horizontal reflections of these functions we will have a sample space consisting of rectangular boxes in $d + 1$ dimensions. This is the crucial point in the Reflection EMCI method. For example, in a bivariate function we may use the following $2^d=4$ Down forms: $f(x,y)$, $f(1-x,y)$, $f(x,1-y)$, $f(1-x,1-y)$. By reflecting these functions horizontally we may get four additional curves: $1-f(x,y)$, $1-f(1-x,y)$, $1-f(x,1-y)$, and $1-f(1-x,1-y)$. Therefore, the integration of a bivariate function will involve eight corners of a three-dimensional rectangular box.

In order to demonstrate the performance of EMCI in higher dimensions we worked on the functions studied in Section 3 by forming their additions for two and three variables.

For example, for the trigonometric function we obtained a bivariate function $f(x,y)$ =sin(x) + sin(y) and a three-variate function $f(x,y, z)$ = sin(x) + sin(y) + sin(z). The average variance reductions of the reflection EMCI estimator for these cases are summarized in Table 10. In d = 2 and d = 3 columns each entry is the mean of eight and 16 values, respectively. The difference between performances of various functions can be attributed to the magnitudes of curve intersections and empty regions. By changing the box dimensions it is possible to improve the performance further.

In higher dimensions the number of function evaluations increases exponentially with d and this creates the curse of dimensionality problem. In this case, using only some evaluations can be recommended. For example, according to our data, in bivariate functions $f(x,y)$ and 1-f(1-x,1-y) are situated on opposite corners and have a minimum intersection. Therefore, their joint usage provides rather good improvement compared to a single function. It is also promising to investigate the suitability of our method to multi-core processors. In this application each form can be assigned to a different core and the results can be collected for final evaluation.

Table 10. Mean ratio obtained by dividing the variances of single Hit-or-Miss estimators to the variance of the Reflection EMCI method

Function	d =2	d =3
Sine	51.4	81.7
Exponential	13.6	11.1
Square root	9.8	9.6
Square	11.8	11.5
Cube	7.5	7.2
Beta	5.5	6.8

8. CONCLUSIONS AND FURTHER RESEARCH

In estimating integrals or finding areas (volumes) of figures (objects) the Hit-or-Miss Monte Carlo method can be used by considering different orientations of the regions. In functions within a unit square, this can be realized by finding the mean value of integrations in different regions created by rotations and reflections. These regions define a multinomial probability distribution and by considering different sub-regions we prove that our proposed method, Extended Monte Carlo Integration, causes a substantial reduction in the variance of the estimate. In the current literature the Hit-or-Miss method has a very restricted application and is considered mainly for historical interest. Our new method creates an estimator with a rather small variance. Its efficiency can be improved further by choosing suitable rectangles other than the unit square in order to minimize intersections or empty regions in the plane. There are cases very common in physics, chemistry, medicine, genetics and biology where there is no explicit function defining the region or the volume to be estimated. These cases are generally restricted to two- and three-dimensional spaces. A distinct advantage of our method is its applicability to these problems. Here, instead of different forms of function expression, various reflections and rotations of the figure or object can be used.

As final remarks we can suggest that:

- The method can be generalized to higher dimensions and non-unit rectangular boxes.

- Since the number of function evaluations increases exponentially with dimension, only some forms taking place on opposite corners may be considered for calculations.

- The parallel calculation possibilities of multi-core computers will be beneficial in speeding up calculations in higher dimensions.

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MONTE CARLO İNTEGRASYONUNDA VARYANS AZALTICI YENİ BİR TEKNİK

ÖZET

Monte Carlo tekniği, rasgele sayılar kullanarak yüzey alanlarını veya cisim hacimlerini bulmaya yarayan bir istatistik deney metodu olarak kullanılabilir. Karmaşık fonksiyonlarda veya düzgün olmayan şekillerde özellikle yüksek boyutlu uzaylar için yararlıdır. Monte Carlo tekniğine yeni bir yaklaşım sunan bu çalışmamızda mültinom dağılıştan hareketle nokta atışlarındaki İsabet-veya- İsabetsizlik integrasyonuna farklı bir bakış açısı getirilmekte ve Genelleştirilmiş Monte Carlo İntegrasyonu diye adlandırdığımız bir teknik tanıtılmaktadır. Burada, tek değişkenli integral işlemi yapılırken, üzerinde çalışılan alanın değişik eğrilerle ifade edilmesiyle elde edilecek farklı tahmin edicilerin ortalaması alınmakta ve böylece hesaplama hızı makul bir sınırda tutulurken, tahminin etkinliği arttırılmaktadır. Birim kare şeklindeki bir düzlemde kullanılan tek değişkenli fonksiyonlar yardımıyla bu yeni tekniğin uygulaması gösterilmiştir. Metod daha yüksek boyutlara da genelleştirilebilir. Öte yandan, fizik, kimya, tıp, genetik ve biyolojide, alanı veya hacmi hesaplanacak yüzey veya şekilleri ifade eden belli bir fonksiyonun bulunmadığı yaygın durumlar vardır. Bu durumlarda farklı fonksiyon ifadeleri yerine, yüzey veya cisim değişik yansımalara ve döndürmelere tabi tutulabilir. Teklif ettiğimiz yeni tekniği üstün kılan seçici özelliklerden birisi, bu tür problemlere uygulanabilmesidir. Metodun çok işlemcili bilgisayar ortamlarına uygulanabilmesi de üzerinde durulmaya değer bir husustur.

Anahtar Kelimeler: Etkinlik, Ham Monte Carlo, İsabet-veya-isabetsizlik integrasyonu, Monte Carlo, Monte Carlo integrasyonu, Rastgele sayı üreticisi, Varyans azaltılması.