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Variance reduction in Monte Carlo for Integrals

Yuchen Yang[1,4,*,†], Jun Zhou[2,5,†], Xiaotong Chen[3,6,†]

[1]School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai, China
[2]Shien-Ming Wu School of Intelligent Engineering, South China University of Technology, Guangzhou, China
[3]College of Media, Sichuan Conservatory of Music, Chengdu, China

[4]3168917147@qq.com
[5]19857417566@163.com
[6]2578291900@qq.com
[*]corresponding author
[†]These authors contributed equally to this work and should be considered co-first authors.

Abstract. Nowadays, the extensive use of Monte Carlo methods in various fields has promoted the scientific decision-making, improved the efficiency of social operation, and enabled better management of many uncertain factors in daily life. However, in some cases, traditional Monte Carlo methods doesn't work so well because of the excessive variance. This paper aims to explore a new numerical integration method called splitting method to minimize intrinsic variance in Monte Carlo simulations. Through this innovative method, we found that the variance was reduced significantly. Despite some oscillating functions which are still difficult to estimate because they have too many turning points, this study provides new insights into variance reduction in Monte Carlo for integrals to optimize calculations in various fields when the modelling functions are not monotonic.

Keywords: Monte Carlo, variance reduction, control variates.

1. Introduction

Monte Carlo methods are used widely in the field of finance, biology, physical sciences and engineering. Its core advantage lies in its ability to handle complex randomness and uncertainty problems, providing more accurate basis for decision-making. However, it also has many drawbacks including high computational costs, slow convergence speed, large sample size requirements, and high dependence on the model. Therefore, to estimate intervals accurately and efficiently, variance reduction is crucial. This paper explores a new numerical integration method called splitting method for reducing intrinsic variance in Monte Carlo simulations. The application of these techniques not only optimizes computing resources but also broadens the applicability of Monte Carlo methods. The paper is divided into five parts: the first part is the introduction of the paper, the second part reviews related work of the applications of Monte Carlo methods in different fields, the third part describes Monte Carlo methods and control variates, the fourth part presents experimental results of various

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functions and proposes the innovative method, and the fifth part draws conclusions and discusses the limitation of this paper.

2. Literature Review

Nowadays, Monte Carlo methods are usually applied in the fields of mathematics and science and can effectively solve various complicated mathematical problems. Maanane et al. used the symbolic Monte Carlo method to identify the radiation characteristics of non-uniform materials, and the polynomials obtained through this method allow for complete inverse analysis, thereby improving efficiency and stability [1]. Meanwhile, Zhou et al. introduced the Monte Carlo method in the stability analysis of the dispersion strength characteristics of soil rock mixtures, effectively improving the accuracy of the stability analysis method [2]. Wicaksono et al. proposed a new paradigm Monte Carlo Fuzzy Hierarchy Analysis (NMCFAHP) by introducing normally distributed fuzzy numbers, which is more effective in overcoming uncertainty in the group decision-making process [3]. In addition, Sangwongwanich et al. developed a Monte Carlo simulation method with incremental damage by considering the cumulative damage of the system, which is suitable for fault-tolerant systems and can be effectively applied in the direction of reliability assessment of power electronic equipment [4]. Moreover, Mongwe et al. proposed a new method for solving the high variance problem in Hamiltonian Monte Carlo (HMC) estimators, including back sampling combined with importance sampling, diamagnetic Hamiltonian Monte Carlo, and diamagnetic momentum Hamiltonian Monte Carlo, to improve posterior inference in machine learning [5]. Afterwards, Sarrut et al. reviewed the ecosystem of the open-source Monte Carlo toolkit GATE for medical physics and introduced the application of Monte Carlo simulation methods in medical physics [6]. Besides, Song et al. provided a more comprehensive exposition of Monte Carlo and variance reduction methods, a thorough review of the relevant formulations and techniques, and an in-depth summary of the development of existing numerical methods, covering general formulations, specific subcategories and their variants, and applications, as well as a comparison of the strengths and weaknesses of different methods [7]. Furthermore, considering the uncertainty of out-of-distribution data prediction, Yelleni et al. proposed the Monte Carlo DropBlock (MC DropBlock) method to simulate the uncertainty in YOLO and the convolutional visual transformer used for object detection, effectively improving the model's generalization ability [8]. And Mazzola, G also analyzed the feasibility of Monte Carlo's application in the field of quantum computing and the future challenges it faces [9]. Monte Carlo methods have already been applied in so many fields, so it is of great practical significance to improve the precision of Monte Carlo methods through variance reduction.

3. Methods

3.1. Monte Carlo Methods

In many applications in mathematics, computing the expectation $E[X]$ of a random variable *X*, e.g., in option pricing or utility maximization theory is often needed. However, it is not always possible to compute $E[X]$ analytically. Therefore, it is crucial to find methods to approximate).

Suppose there is a sequence of random variables (X_i), which are mutually independent and identically distributed with the same distribution as *X*. Then, with probability one, we have

$$\frac{1}{n}\sum_{i=1}^{n} X_i \rightarrow E[X], \qquad (n \rightarrow \infty). \tag{1}$$

by the so-called *Strong Law of Large Numbers (SLLN)*, which turns a sequence of random observations into a deterministic number by computing the average.

If many independent realizations are generated from the same distribution, and these realizations are averaged, by the *SLLN*, it is sure that for large n the average is close to the true expected value, which is called Monte Carlo methods. Monte Carlo methods stem from the analogy between probability and volume and calculate the volume of a set by interpreting the volume as a probability.

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In the simplest case, this means randomly sampling from a range of possible outcomes and selecting a portion from a given set as an estimate of the volume of that set. The law of large numbers ensures that as the number of draws increases, the estimate value will converge to the correct value. The central limit theorem provides information on the possible size of estimation errors after finite drawing [10].

Monte Carlo method algorithms can be summarized as the following pattern:

1.Define a possible input domain

2.Generate inputs randomly based on the probability distribution on the domain

3.Perform a deterministic calculation of the outputs

4.Sum up the results

In principle, Monte Carlo methods can be used to solve any problem with probabilistic explanations. However, a major limitation of Monte Carlo methods is their high dependence on sample size. For example, let's evaluate $\int_0^1 x^2 dx$.

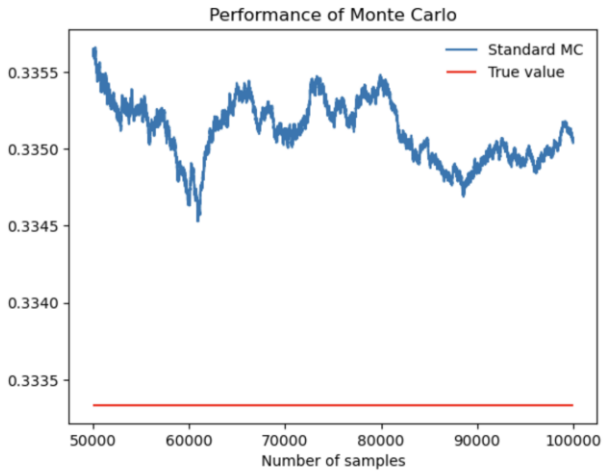

Figure 1. Performance of Monte Carlo when evaluate $\int_0^1 x^2\, dx$.

As figure 1 shows, even if the sample size in Monte Carlo simulation is large enough, it is impossible to estimate a perfect fit with the correct value because the accuracy of Monte Carlo estimation is limited by the random distribution and integral characteristics of the samples.

3.2. Control Variates

The method of control variates is one of the most effective and widely applicable techniques to improve the efficiency of Monte Carlo simulations. It utilizes the information of known quantity estimation error to realize error decreasing of unknown quantity estimation [10].

The control-variates method for estimating $E[X]$ can be described as follows.

Suppose the pairs $(X_i,\ Y_i)$, $i = 1, \dots, n$ are independent and identically distributed, and that the expectation $E[Y]$ is known. The control-variates estimator with b^* of $E[X]$ is defined by

$$\overline{X_n}(b) := \overline{X_n} - b(\overline{Y_n} - E[Y]) = \frac{1}{n}\sum_{i=1}^{n}(X_i - b(Y_i - E[Y])) \tag{2}$$

Note that the observed error $\bar{Y}_n$ - $E[Y]$ is used to control the estimation of $E[X]$.

The mean of the control-variates estimator is

$$E[\overline{X_n}(b)] = \frac{1}{n}\sum_{i=1}^{n} E[X_i(b)] = E[X], \tag{3}$$

so, it's unbiased. The variance of the control-variates estimator is

$$\mathrm{Var}\big(\overline{X_n}(b)\big) = \frac{1}{n^2}\sum_{i=1}^{n} \mathrm{Var}\big(X_i(b)\big) \tag{4}$$

$$= \frac{1}{n}\mathrm{Var}\big(X_i(b)\big) \tag{5}$$

$$= \frac{1}{n}\big(\mathrm{Var}(X) - 2b\mathrm{Cov}(X,Y) + b^2\,\mathrm{Var}(Y)\big) \tag{6}$$

This variance is a function in b, and we want to minimize it with respect to b. By setting the derivative in b equal to zero we can get the value b^* which minimizes the variance. This value is given by

$$b^* = \frac{\mathrm{Cov}(X,Y)}{\mathrm{Var}(Y)} \tag{7}$$

Substituting b^* for b in (6), we obtain

$$\mathrm{Var}\big(\overline{X_n}(b^*)\big) = \frac{1}{n}\left(\mathrm{Var}(X) - \frac{\mathrm{Cov}(X,Y)^2}{\mathrm{Var}(Y)}\right). \tag{8}$$

This expression and the fact that

$$\mathrm{Var}(\overline{X_n}) = \frac{1}{n}\mathrm{Var}(X) \tag{9}$$

imply that

$$\frac{\mathrm{Var}\big(\overline{X_n}(b^*)\big)}{\mathrm{Var}(\overline{X_n})} = 1 - \frac{\mathrm{Cov}(X,Y)^2}{\mathrm{Var}(X)\mathrm{Var}(Y)} = 1 - {\rho_{XY}}^2 \tag{10}$$

where ρ_{XY} is the correlation between X and Y. The control variates method is useful provided that the squared correlation ${\rho_{XY}}^2$ of X and Y is large and the extra computational effort associated with generating the samples Y_i is relatively small.

4. Results

4.1. Experiments of basic functions

Let's try different basic functions, including exponential functions, power functions, logarithmic functions, trigonometric functions and inverse trigonometric functions, and compare the performance of control variates with Monte Carlo.

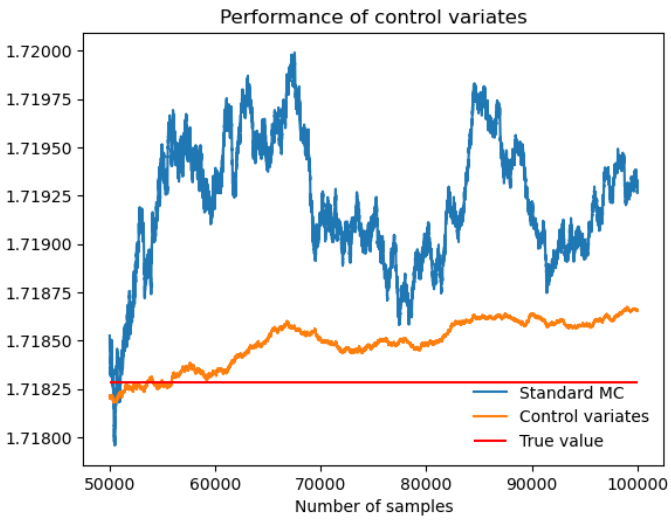

Figure 2. Performance of control variates compared with Monte Carlo when evaluate $\int_0^1 e^x\,dx$.

Table 1. $\int_0^1 e^x \, dx$.

Actual value of integral	1.7183
Standard MC estimate (b = 0)	1.7193
MC standard deviation	0.00156
Control-variates estimate with b = b*	1.7187
Control-variates standard deviation	0.00020
Variance reduction (empirical)	0.98

As figure 2 and table 1 show, the performance of control variates is much better than Monte Carlo with an empirical variance reduction of about 98%.

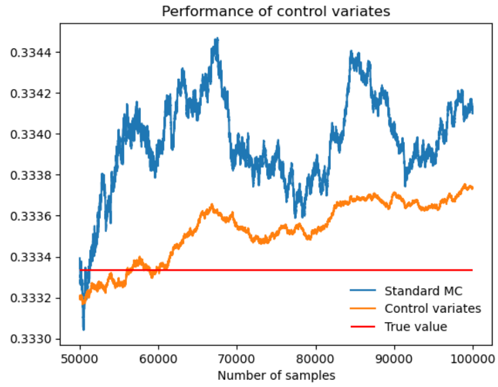

Figure 3. Performance of control variates compared with Monte Carlo when evaluate $\int_0^1 x^2 \, dx$.

Table 2. $\int_0^1 x^2 \, dx$.

Actual value of integral	0.3333
Standard MC estimate (b = 0)	0.3341
MC standard deviation	0.00095
Control-variates estimate with b = b*	0.3337
Control-variates standard deviation	0.00024
Variance reduction (empirical)	0.94

As figure 3 and table 2 show, the performance of control variates is much better than Monte Carlo with an empirical variance reduction of about 94%.

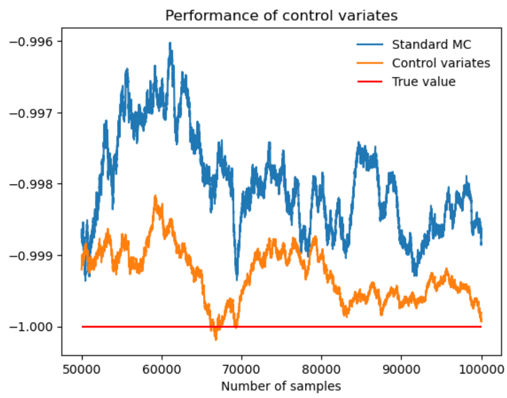

Figure 4. Performance of control variates compared with Monte Carlo when evaluate $\int_0^1 \ln x \, dx$.

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Table 3. $\int_0^1 \ln x \, dx$.

Actual value of integral	-1.0000
Standard MC estimate (b = 0)	-0.9988
MC standard deviation	0.00316
Control-variates estimate with b = b*	-0.9999
Control-variates standard deviation	0.00158
Variance reduction (empirical)	0.75

As figure 4 and table 3 show, the performance of control variates is better than Monte Carlo with an empirical variance reduction of about 75%.

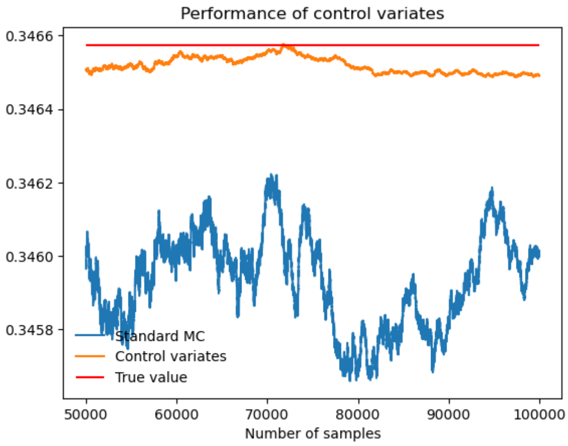

Figure 5. Performance of control variates compared with Monte Carlo when evaluate $\int_0^{\frac{\pi}{4}} \tan x \, dx$.

Table 4. $\int_0^{\frac{\pi}{4}} \tan x \, dx$.

Actual value of integral	0.3466
Standard MC estimate (b = 0)	0.3460
MC standard deviation	0.00069
Control-variates estimate with b = b*	0.3465
Control-variates standard deviation	0.00006
Variance reduction (empirical)	0.99

As figure 5 and table 4 show, the performance of control variates is much better than Monte Carlo with an empirical variance reduction of about 99%.

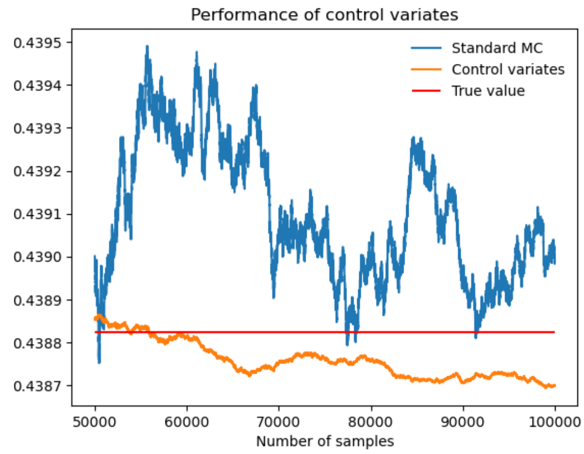

Figure 6. Performance of control variates compared with Monte Carlo when evaluate $\int_0^1 \tan^{-1} x\, dx$.

Table 5. $\int_0^1 \tan^{-1} x\, dx$.

Actual value of integral	0.4388
Standard MC estimate (b = 0)	0.4390
MC standard deviation	0.00073
Control-variates estimate with b = b*	0.4387
Control-variates standard deviation	0.00007
Variance reduction (empirical)	0.99

As figure 6 and table 5 show, the performance of control variates is much better than Monte Carlo with an empirical variance reduction of about 99%. In conclusion, when the functions are monotonic, the effect of variance reduction is usually significant.

4.2. Experiments of other functions

When it comes to double integrals, control variates also work. It is noteworthy that the choosing of variable functions is essential because different variable functions have different correlations and result in different variance reduction. As figure 7 and table 6 show, when the integrand is $e^x * e^y$, there is no remarkable difference between the results of the two variable functions.

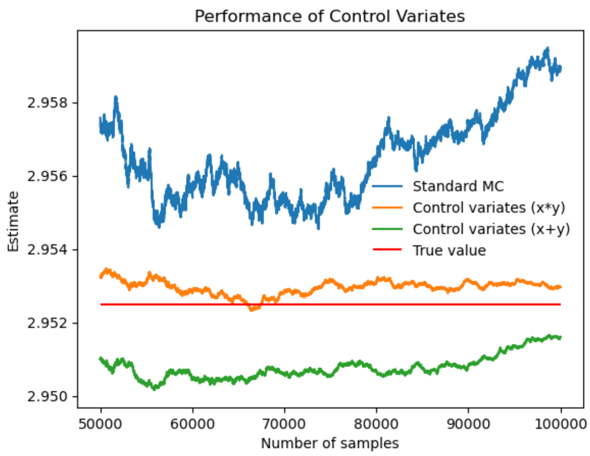

Figure 7. Performance of control variates (*x***y*) compared with control variates (*x*+*y*) and Monte Carlo when evaluate $\iint_0^1 e^x * e^y\, dx\, dy$.

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Table 6. $\iint_0^1 e^x * e^y \, dx \, dy$.

variable g (x, y)	$x*y$	$x+y$
Correlation	0.9735	0.9722
Actual value of integral	2.9525	2.9525
Standard MC estimate (b = 0)	2.9589	2.9589
Monte Carlo standard deviation	0.00385	0.00385
Control-variates estimate with b = b*	2.9530	2.9516
Control-variates standard deviation	0.00088	0.00090
Variance reduction (empirical)	0.947	0.945

However, when the integrand is e^{xy}, as figure 8 and table 7 show, it is obvious that $x*y$ is a better option than $x+y$ when selected variable functions, because in this case where x and y are both between 0 and 1, $x*y$ is smaller than $x+y$.

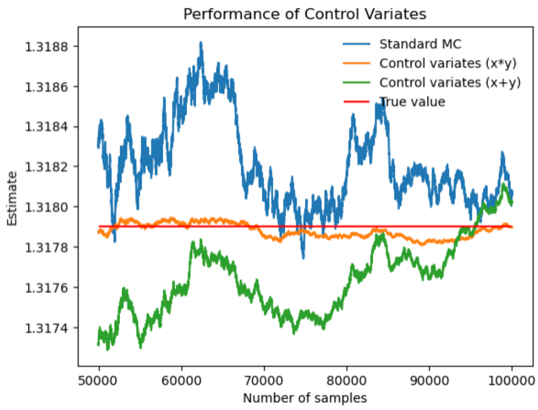

Figure 8. Performance of control variates ($x*y$) compared with control variates ($x+y$) and Monte Carlo when evaluate $\iint_0^1 e^{xy} \, dx \, dy$.

Table 7. $\iint_0^1 e^{xy} \, dx \, dy$.

variable g (x, y)	$x*y$	$x+y$
Correlation	0.9921	0.8969
Actual value of integral	1.3179	1.3179
Standard MC estimate (b = 0)	1.3181	1.3181
Monte Carlo standard deviation	0.00103	0.00103
Control-variates estimate with b = b*	1.3179	1.3180
Control-variates standard deviation	0.00013	0.00045
Variance reduction (empirical)	0.98	0.80

Speaking of functions with infinite intervals, as figure 9 and table 8 show, control variates don't perform well, with only 0.119708 in variance reduction.

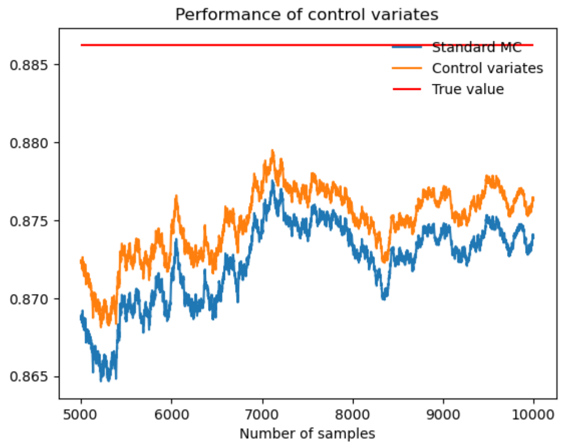

Figure 9. Performance of control variates compared with Monte Carlo when evaluate $\int_0^\infty e^{-x^2}\,dx$.

Table 8. $\int_0^\infty e^{-x^2}\,dx$.

Actual value of integral	0.8862
Standard MC estimate (b = 0)	0.8739
Monte Carlo standard deviation	0.01010
Control-variates estimate with b = b*	0.8763
Control-variates standard deviation	0.00947
Variance reduction (empirical)	0.12

4.3. Splitting method

The functions discussed above are all monotonic functions. Let's discuss functions that are not monotonic. If control variates are used directly, their performance is terrible, which act the same as standard Monte Carlo. But if the function is split into two parts, which are respectively monotonic, and then sum them up, the performance of control variates will improve a lot. This innovative method is called splitting method, and the performance of this new method is called control variates+.

For example, let's evaluate $\int_0^1 (x-\frac{1}{2})^2\,dx$.

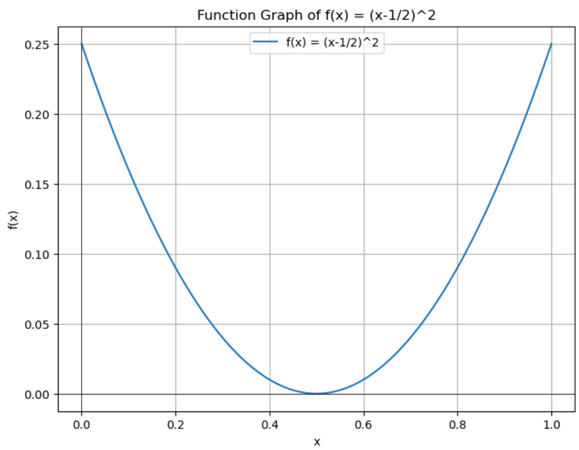

Figure 10. Function graph of $(x-\frac{1}{2})^2$

Figure 10 shows the function graph of $(x-\frac{1}{2})^2$.

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First, let's directly evaluate $\int_0^1 (x-\frac{1}{2})^2\,dx$.

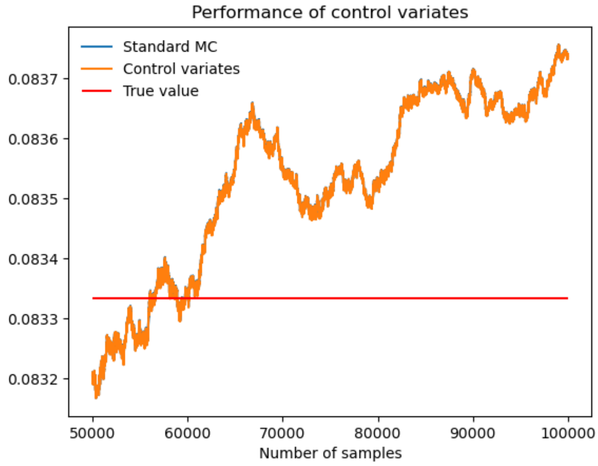

Figure 11. Performance of control variates compared with Monte Carlo when evaluate $\int_0^1 (x-\frac{1}{2})^2\,dx$.

Table 9. $\int_0^1 (x-\frac{1}{2})^2\,dx$.

Actual value of integral	0.0833
Standard MC estimate (b = 0)	0.0837
Monte Carlo standard deviation	0.00024
Control-variates estimate with b = b*	0.0837
Control-variates standard deviation	0.00024
Variance reduction (empirical)	0.000044

As figure 11 and table 9 show, control variates and standard MC almost overlap and the variance reduction is only 0. 000044, which means in this case, control variates are nearly useless. Then, let's split the integration interval into two monotonic subintervals and estimate independently in each subinterval.

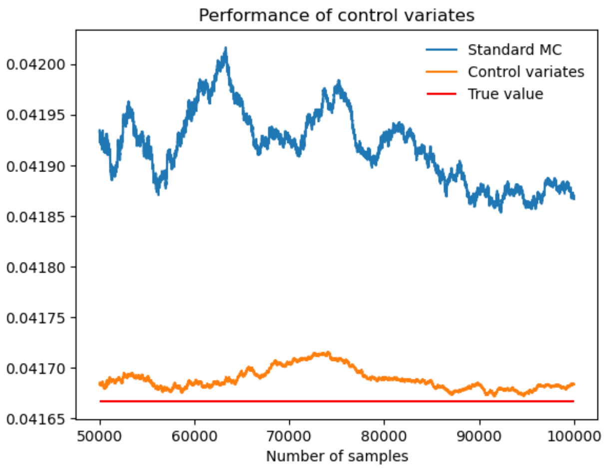

Figure 12. Performance of control variates compared with Monte Carlo when evaluate $\int_0^{\frac{1}{2}} (x-\frac{1}{2})^2\,dx$.

Table 10. $\int_0^{\frac{1}{2}}(x-\frac{1}{2})^2\,dx.$

Actual value of integral	0.04167
Standard MC estimate (b = 0)	0.04187
Monte Carlo standard deviation	0.00012
Control-variates estimate with b = b*	0.04168
Control-variates standard deviation	0.00003
Variance reduction (empirical)	0.94

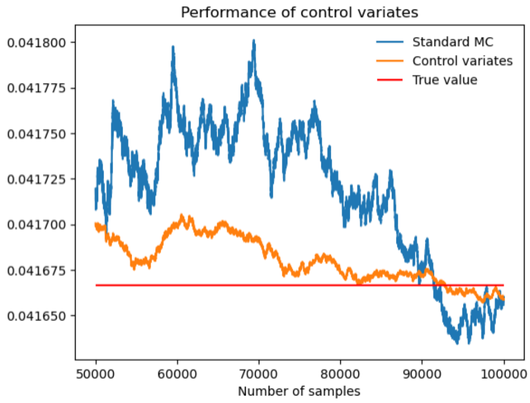

Figure 13. Performance of control variates compared with Monte Carlo when evaluate $\int_{\frac{1}{2}}^{1}(x-\frac{1}{2})^2\,dx.$

Table 11. $\int_{\frac{1}{2}}^{1}(x-\frac{1}{2})^2\,dx.$

Actual value of integral	0.04167
Standard MC estimate (b = 0)	0.04167
Monte Carlo standard deviation	0.00012
Control-variates estimate with b = b*	0.04167
Control-variates standard deviation	0.00003
Variance reduction (empirical)	0.94

As figure 12,13 and table 10,11 show, both the two monotonic subintervals perform well. After that, let's sum the two results up and obtain the final integral estimate.

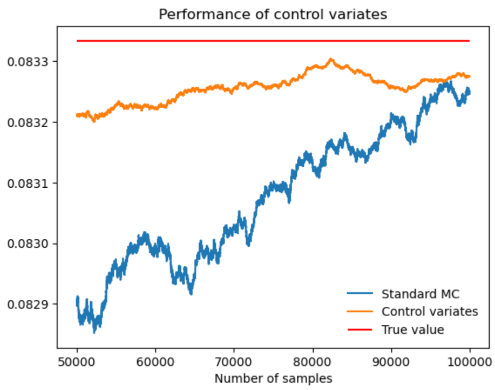

Figure 14. Performance of control variates compared with Monte Carlo when evaluate $\int_0^{\frac{1}{2}}(x-\frac{1}{2})^2\,dx+\int_{\frac{1}{2}}^{1}(x-\frac{1}{2})^2\,dx.$

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Table 12. $\int_0^{\frac{1}{2}}(x-\frac{1}{2})^2\,dx+\int_{\frac{1}{2}}^{1}(x-\frac{1}{2})^2\,dx.$

Actual value of integral	0.08333
Standard MC estimate (b = 0)	0.08325
Monte Carlo standard deviation	0.00024
Control-variates estimate with b = b*	0.08328
Control-variates standard deviation	0.00006
Variance reduction (empirical)	0.94

As figure 14 and table 12 show, the final integral estimate performs well. Finally, let's compare the results of control variates with and without splitting method.

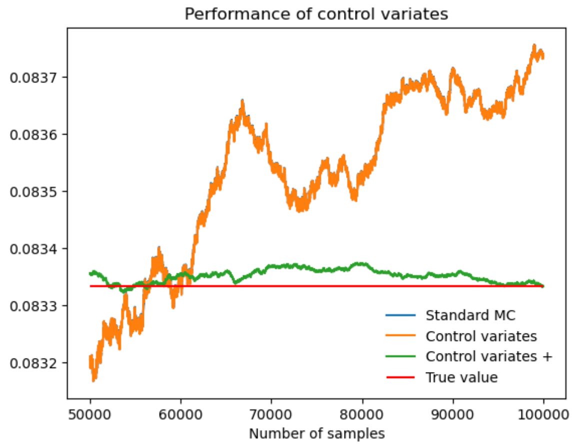

Figure 15. Performance of control variates+ compared with control variates and Monte Carlo when evaluate$\int_0^1(x-\frac{1}{2})^2\,dx$.

As figure 15 shows, it is evident that control variates+ have a much better performance than control variates. Likewise, as figure 16 shows, integrals like $\int_0^{\pi}\sin x\,dx$ can also be estimated by splitting method, solving the problem that control variates are useless to estimate integrals with turning points.

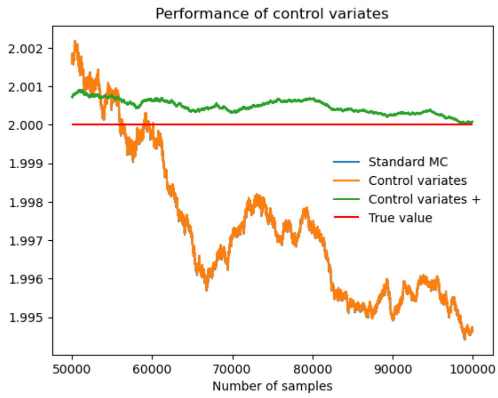

Figure 16. Performance of control variates+ compared with control variates and Monte Carlo when evaluate$\int_0^{\pi}\sin x\,dx$.

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5. Conclusion

This paper proposes a new numerical integration strategy, which splits the integration interval into several monotonic subintervals and estimate the control variables independently in each subinterval and then the results of each segment can be summed up to obtain the final integral estimate. Such methods minimize the variance inherent in Monte Carlo simulations and improve the accuracy and efficiency of numerical integral estimates. Although the splitting method can solve the problem of estimating the integrals of non-monotonic functions, some oscillating functions, like $\sin x$ and $\cos x$, have too many turning points to split, which requires a lot of splitting. And if the splitting method is not used, the direct control variates is almost useless. Therefore, when encountering a function with too many oscillations, variance reduction in Monte Carlo may not help so much.

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All authors contributed equally to this work and should be considered co-first authors.

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