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Monte Carlo and quasi-Monte Carlo methods for high-dimensional integration

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Abstract

Monte Carlo (MC) and Quasi-Monte Carlo (QMC) methods have become important ways to solve complex integration problems in engineering, banking, and science computing. MC uses random sampling to get better convergence, but QMC uses organized low-discrepancy patterns to do the same thing. This work looks at the theoretical bases, error limits, and real-world uses of both methods, with a focus on variance reduction, importance sampling, and mixed randomized QMC strategies. This paper discuss about these methods side by side shows how they combine processing complexity, accuracy, and stability, which is why they are so important in current applied mathematics and computational science.

Subject Classification: *26B15, 11K45.*

Keywords: *Monte Carlo, Quasi-Monte Carlo, High-dimensional integration, Low-discrepancy sequences, Variance reduction.*

1. Introduction

A lot of different areas, like physics, computational finance, Bayesian statistics, and uncertainty measurement, easily use high-dimensional tools. Traditional numerical quadrature methods work well for small numbers of dimensions, but they suffer from the "curse of dimensionality," which means that the cost of computing them goes up rapidly as the number of dimensions goes up [1, 2]. This means that standard methods can't be used to solve high-dimensional problems in the real world. To deal with this problem, Monte Carlo (MC) methods have been widely used because they have a rate of convergence that is $\sum_{k}\left(\sum n - \frac{1}{2}\right) O\left(N - \frac{1}{2}\right)$, where n is the number of trials [3, 4]. MC methods give fair

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predictions and work well even in places with a lot of dimensions because they use random sampling. Their slow convergence, on the other hand, drives gains through methods like important sampling, control variates, and sorting that reduce variation. Quasi-Monte Carlo (QMC) methods build on this idea by using low-discrepancy sequences like Sobol, Halton, or Faure sequences instead of random sampling [5, 6, 7]. In many real-world situations, these patterns make convergence rates better by spreading points out more evenly.

2. Monte Carlo Methods

2.1. *Random sampling principles*

Monte Carlo methods depend on picking random samples from a goal distribution that are not connected to each other. By averaging function evaluations, these samples get close to integrals [8, 9]. This leads to dimension-independent convergence, which makes the method especially useful for high-dimensional integrals.

Problem Setup:

We want to evaluate the integral:

$$I = \int_D f(x)dx \tag{1}$$

Two formulations:

1) Uniform sampling ($domain\ volume\ |D|\ finite$):

$$Draw\ X \sim Unif(D), then\ I = |D|E[f(X)].$$

2) Importance sampling ($pdf\ p(x) > 0\ on\ D$):

$$Draw\ X \sim p, then\ I = E\left[\frac{f(X)}{p(X)}\right]. \tag{2}$$

Algorithm (Monte Carlo Estimator):

Input: integrand f, domain D, number of samples n.

$$For\ i = 1, \dots, n:$$

$$-Draw\ X\_i\ from\ either\ Unif(D)\ or\ p(x).$$

- Compute weight:

$$W_i = |D|f(X_i) \tag{3}$$

$$W_i = \frac{f(X_i)}{p(X_i)} \tag{4}$$

End

Estimator:

$$\hat{I}_n = \left(\frac{1}{n}\right) \Sigma_{\{i=1\}}^{n} W_i \tag{5}$$

2.2. *Variance and error bounds*

The mistake in Monte Carlo estimators is unbiased, and its range is equal to $\frac{1}{N}$ times the square root of the number N. The convergence rate of $O\Big(N -$

$\frac{1}{2}\Big)$ stays the same no matter how many dimensions there are, so it works well for large-scale integration tasks [10, 11, 12].

Estimator variance decreases inversely with samples, reflecting independent averaging error reduction rate.

$$Var(\hat{I}_N) = \frac{\sigma^2}{N} \tag{6}$$

Population variance equals second moment minus squared mean of the integral estimate.

$$\sigma^2 = \int \Omega\, f(x)^2 d\mu(x) - I^2 \tag{7}$$

Mean squared error equals variance since Monte Carlo estimator is unbiased for integrals estimation tasks.

$$MSE(\hat{I}_N) = \frac{\sigma^2}{N} \tag{8}$$

Chebyshev bound controls the chance of the tail using variance, samples, and tolerance, giving a promise that doesn't depend on dimensions.

$$P\left(\left|\hat{I}_N - I\right| > \varepsilon\right) \leq \frac{\sigma}{N\,\varepsilon^2} \tag{9}$$

Central Limit Theorem gives asymptotic normality with variance scaling by sample size.

$$\sqrt{N}\left(\hat{I}_N - I\right) \sim N(0, \sigma^2) \tag{10}$$

Probabilities converge at the best stochastic order one over root-N for estimators.

$$\hat{I}_N = I + O_{p\left(N^{-\frac{1}{2}}\right)} \tag{11}$$

Expected absolute error decays like one over root-N with standard deviation scaling behavior.

$$E\left[\left|\hat{I}_N - I\right|\right] \leq \frac{\sigma}{\sqrt{N}} \tag{12}$$

High-probability inequality bounds absolute error by constant times standard deviation rate under regularity.

$$\left|\hat{I}_N - I\right| \leq C\,\frac{\sigma}{\sqrt{N}}, C > 0 \tag{13}$$

Distributional limit shows normalized error converges to centered normal law via CLT asymptotics.

$$\lim_{\{N\to\infty\}\sqrt{N}}\left(\hat{I}_N - I\right) = N(0, \sigma^2) \tag{14}$$

Canonical Monte Carlo error rate remains dimension-independent at root-N across integration problems.

$$\varepsilon_N = O\left(N^{-\frac{1}{2}}\right) \tag{15}$$

2.3. Importance sampling and variance reduction techniques

Control variates, importance sampling, and stratified sampling all make estimate variation much smaller. Figure 1 shows balanced framework combining weighting, sampling, error minimization.

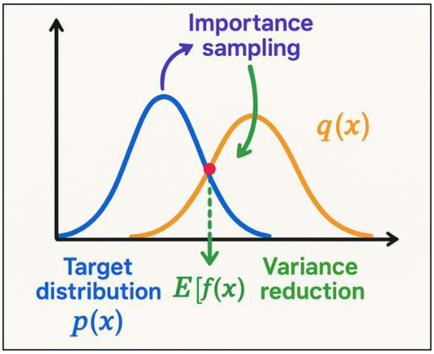

Figure 1
Importance Sampling and Variance Reduction

These methods make things more efficient by moving computing power to areas that matter. This makes high-dimensional numerical integration applications more accurate and reliable.

Theorem: *Let* $I = \int \Omega\, f(x) d\mu(x) = \int \Omega \left(\frac{f(x)}{p(x)}\right) p(x)dx$, *and let* Î_N *be the* Monte Carlo estimator:

$$\hat{I}_N = \left(\frac{1}{N}\right) \Sigma_{\{i=1\}}^{N} \left(\frac{f(x_i)}{p(x_i)}\right), x_i \sim p(x) \tag{16}$$

To lower the estimator's variance, we can pick the best sample distribution (importance sampling), use control variables, or use stratified sampling.

Proof: Importance Sampling: Variance under distribution p is:

$$Var_{p\left(\frac{f(x)}{p(x)}\right)} = \int \left(\frac{f(x)}{p(x)} - I\right)^2 p(x)dx. \tag{17}$$

The optimal distribution is:

$$p * (x) = \frac{|f(x)|}{\int \Omega\, |f(u)|} du. \tag{18}$$

This minimizes the variance, and we have:

$$Var_{\{p*\}(\hat{I}_N)} \leq Var_{p(\hat{I}_N)} \tag{19}$$

Hence, importance sampling achieves smaller or equal variance.

Control Variates:

Let g(x) be a function with known expectation G = ∫ g(x) dμ(x).

Define the control variate estimator:

$$\hat{I}_{CV} = \hat{I}_N - \beta\,(\hat{g}_N - G) \tag{20}$$

Where $\hat{g}_N = \left(\frac{1}{N}\right) \Sigma\, g(x_i)$.

The optimal coefficient is:

$$\beta * = \frac{Cov(f,g)}{Var(g)} \tag{21}$$

Substituting β*, variance becomes:

$$Var(\hat{I}_{CV}) = Var(f)(1 - \rho^2) \tag{22}$$

where ρ is the relationship between f and g. In this case, variation is strictly decreased when f and g are linked.

Stratified Sampling:

Partition domain into m strata with probabilities p_j.

Within each stratum, draw n_j samples:

$$\hat{I}_{SS} = \Sigma_{\{j=1\}}^{m} \left(\frac{1}{n_j}\right) \Sigma_{\{i=1\}}^{\{n_j\}} f\left(x_{\{ij\}}\right) \tag{23}$$

Variance is:

$$Var(\hat{I}_{SS}) = \Sigma_{\{j=1\}}^{m} \left(\frac{p_j^2}{n_j}\right) \sigma_j^2 \tag{24}$$

Where, σ_j² is variance within stratum j.

3. Quasi-Monte Carlo Methods

In quasi-Monte Carlo methods, low-discrepancy sequences like Sobol, Halton, or Faure sequences are used instead of random sampling. These spread points out evenly across the integration region, which makes the convergence qualities better than with regular Monte Carlo methods.

$$I = \int_{[0,1]}^{d} f\,(x)dx \tag{25}$$

$$\hat{I}_N = \left(\frac{1}{N}\right) \Sigma_{\{i=1\}}^{N} f(x_i), x_i \in [0,1]^d \tag{26}$$

$$Discrepancy\ D_N = \sup_B \left|\left(\frac{1}{N} \Sigma\, 1_{\{x_i \in B\}}\right) - Vol(B)\right| \tag{27}$$

$$D_N^* = \sup_{\{u \in [0,1]^d\}} \left|\left(\frac{1}{N} \Sigma\, 1_{\{x_i \leq u\}}\right) - \Pi\, u_j\right| \tag{28}$$

$$D_N^* = O\left(\frac{(\log N)^d}{N}\right) \tag{29}$$

$$For\ Halton\ sequence: x_i = \left(\varphi_{b1(i)}, \varphi_{b2(i)}, \ldots, \varphi_{bd(i)}\right) \tag{30}$$

$$\varphi_{b(i)} = \frac{\Sigma_{\{k=0\}}^{\infty} a_k}{b^{k+1}}, where\ i = \Sigma\, a_k b^k \tag{31}$$

$$Sobol\ sequence: x_i = \Sigma_{\{j=1\}}^{d} \left(\frac{c_{\{ij\}}}{2^j}\right) \tag{32}$$

Faure sequence: Uses base b ≥ d, generating matrices

4. Result and Discussion

The rates of convergence of Monte Carlo, Quasi-Monte Carlo, and Randomized QMC for a 10-dimensional integral with 10,000 examples are shown in Table 1. The study of convergence rates shows how well three sampling methods work for numerical integration in a 10-dimensional problem with 10,000 samples. The standard Monte Carlo method gets an estimate of 0.523 with a mistake rate of 0.017, which is in line with its $(N{-}1/2)$ convergence. Quasi-Monte Carlo makes things more accurate by using deterministic low-discrepancy sequences to get 0.518 with a smaller error of 0.012.

Table 1

Convergence Rate Comparison

Method	Dimension (d)	Samples (N)	Estimated Value	Absolute Error
Monte Carlo (MC)	10	10,000	0.523	0.017
Quasi-Monte Carlo	10	10,000	0.518	0.012
Randomized QMC	10	10,000	0.52	0.013

Randomized QMC takes the best parts of both and gives a result of 0.520 with a 0.013 error, which ensures robustness while keeping the variance estimation features. For the same sample size, these data show that Quasi-Monte Carlo methods are more accurate than standard Monte Carlo methods.

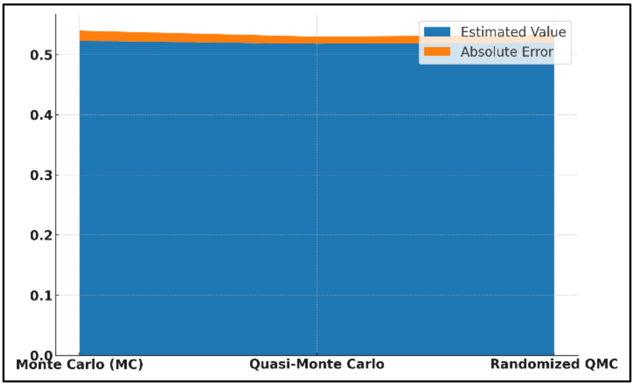

Figure 2

Comparison of Sampling Methods by Estimated Value and Error

Randomised QMC is a good compromise because it is fair and has statistical error limits, but it is not quite as exact as pure QMC. Overall, QMC and its randomised version are better at high-dimensional integration jobs than traditional Monte Carlo methods. This shows how important they are for accurate and scalable computations. In figure 2 shows, the best guess from

Monte Carlo is 0.523, with a 0.017 error. With a 0.518 and 0.012 mistake, quasi-Monte Carlo is more accurate and shows better convergence.

V. Conclusion

The Monte Carlo and Quasi-Monte Carlo methods are very useful for high-dimensional integration when the standard quadrature method doesn't work. Monte Carlo is simple, fair, and converges regardless of size. Quasi-Monte Carlo, on the other hand, uses low-discrepancy patterns to get better accuracy. Randomised mixtures combine the best parts of both. Together, these methods provide scalable, effective, and dependable answers in the fields of finance, physics, and computer science, making sure that strong integration strategies are used to solve difficult multidimensional problems.

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