Monte-Carlo Methods for Definite Integration

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1 Motivation

Monte-Carlo methods are a series of non-deterministic techniques which use random sampling to *approximate* a numerical result. The use of Monte-Carlo methods has many applications to computer science and mathematics. The outlined techniques have unique advantages over common deterministic approximations.

2 Monte-Carlo Methods

2.1 PI Approximation

In-order to unserstand the use of Monte-Carlo methods for definite integration, we will first look at approximating PI with random sampling.

It is known that the area of a circle is πr^2. The area of a square can also be derived, in terms of its radius r, as $4r^2$. Now imagine we were to place a circle inside of a

square, who both happen to share the same length in diameter. Let the ratio of area's be defined as P:

$$\begin{aligned} P &= \frac{\pi r^2}{4r^2} \\ &= \frac{\pi}{4} \end{aligned}$$

Therefore, we can get an approximation of PI as $P = 4 * \frac{\pi}{4}$

A more mathematically rigorous definition of this approximation can be seen with function $P^N(x)$:

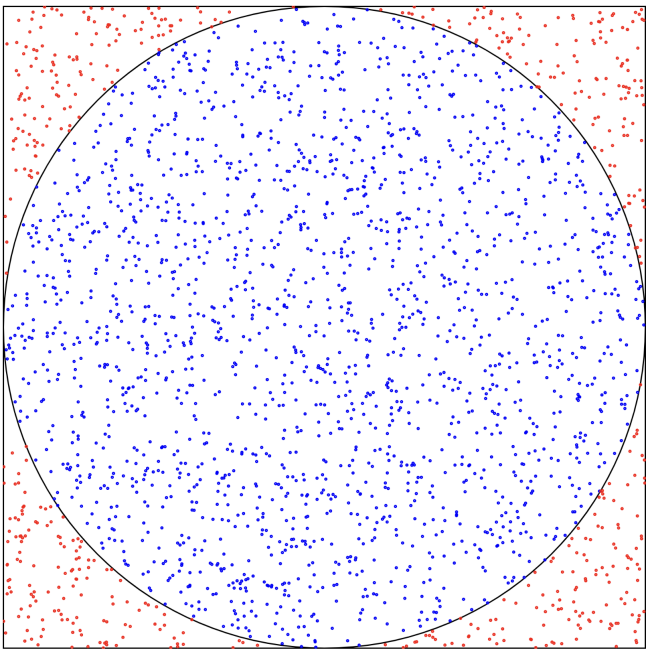
$$P^N = 4\frac{1}{N}\sum_{i=1}^{N} f(x_i, y_i)$$

With $f(x, y)$:

$$\begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$$

Using n random points within the square we can get an approximation of PI P^n. As the sample size n increases, we see a better approximation of PI.

Figure 1: Visual of Random Sampling for PI Approximation



2.2 Monte-Carlo Estimator

We may now apply our understanding of Monte-Carlo methods for PI approximation to its use for approximating definite integrals.

Monte-Carlo integration uses uniform random sampling to compute regions of a function within a given interval. The general idea behind Monte-Carlo integration is to take a random point $X_i \in [a, b]$ and compute $f(X_i)$. We may then take that value and multiply it by $(b - a)$ to form a rectangle of width $(b - a)$ and height $f(X_i)$. The average of all rectangles is our integral approximation.

The Monte-Carlo estimator M^n can be seen as

$$M^N = (b - a)\frac{1}{N - 1}\sum_{i=0}^{N} f(X_i)$$

Where N is the number of random samples. It is important to note that X_i is a random number $\in [a, b]$, with ξ being $\xi[0, 1)$ such that

$$X_i = a + \xi_i(b - a)$$

Therefore our true Monte-Carlo estimator can be seen as

$$M^N = (b - a)\frac{1}{N - 1}\sum_{i=0}^{N} f(a + \xi_i(b - a))$$

3 Variance within Monte-Carlo Integration

When working with random sampling, statistical variance is used to analyze the significance of our approximation, and its deviation from the true integral.

The easiest way to reduce varience is to increase the sample size. As sample size increases to N $= 8,765,000$, the Monte Carlo estimate will be within $\delta = 0.0005$ units of the true value of the integral.[1]

3.1 Error Analysis Through Statistical Techniques

To look at the error that occours with random sampling used in Monte-Carlo integration, we must first define two functions.

The *cumulative distribution function* CDF, of a random variable x, represents the probability of that value to be within a certain threshhold or boundary.

$$cdf(x) = Pr\{X \leq x\}$$

Note that the CDF is always monotonically increasing.

Similarly, the *probability density function* PDF, is the derivitive of CDF. Because the CDF is always monotonically increasing, it is the case that PDF is always > 0.

$$pdf(x) = \frac{d}{dx}cdf(x)$$

[1] https://blogs.sas.com/content/iml/2021/04/05/sample-size-monte-carlo-integral.html

With this knowledge, we can compute the *expected value* of a random variable $Y = f(x)$ to be

$$expect[Y] = \int_a^b f(x)pdf(x)\,dx$$

Furthermore, we can use our computation of $expect[Y]$ to compute the variance. With respect to random variables, the variance is the degree to which the values of a random variable differ from the expected value. [2]

$$\sigma^2[Y] = expect[(Y - expect[Y])^2]$$

Finally, it can be proven that the error term for Monte-Carlo integration is

$$\frac{\sigma^2}{N}[Y]$$

with N being the sample size.

Looking further, the square root of our error term gives us the standard deviation

$$\frac{\sigma}{\sqrt{N}}[Y]$$

Which shows that the Monte-Carlo integral converges with $O(\sqrt{N})$.

4 Variance Reducing Techniques

There are a number of techniques to be unes in combination with Monte-Carlo intregration that aim to reduce the variance in our approximations. The premise behind most of these techniques is to place more samples in strategic areas of the function to yeild more accurate approximations.

4.1 Stratified Sampling

Stratified sampling divides the interval of the integral into N sub-lengths. This allwos for more isolated random sampling within each of the sub-intervals, similar to techniques used by a deterministic Riemann sum. It must be noted that the use of stratified sampling requires a preexisting knowledge of the sample size.

It is neccisary to alter our M^N Monte-Carlo estimator M^N to take advantage of this approach. Since we will divide our interval into N subsections we can see that M^N becomes:

$$\begin{aligned} M^N &= (b-a)\frac{1}{N-1}\sum_{i=0}^{N} f(X_i) \\ &= (b-a)\frac{1}{N-1}\sum_{i=0}^{N} f(a + \frac{i+\xi}{N}(b-a)) \end{aligned}$$

[2] https://nzmaths.co.nz/category/glossary/variance-discrete-random-variable

Figure 2: Visual of Stratified Sampling vs Riemann sum

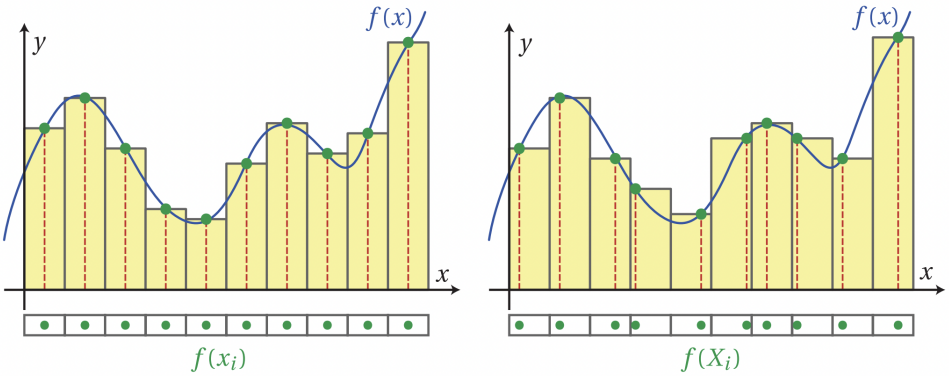


Figure A.3: Deterministic quadrature techniques such as a Riemann summation (left) sample the function at *regular* intervals. Conceptually, stratified Monte Carlo integration (right) performs a very similar summation, but instead evaluates the function at a *random* location within each of the strata.

It is shown that the variance of stratified sampling is never greater than general random sampling. Furthermore, the error seen with stratified sampling reduces linearly with the number of samples.[3]

4.2 Adaptive Sampling

Adaptive sampling attempts to place an increased number of random points in specific and intentional locations along the function. The goal is to yeild greater accuracy in regious of the graph that might normally be challenging to compute the intergral of. This is done while the function is being computed, esentially *on the spot* in areas of high variance.

Implementations are similar to what has been seen during our Numerical Method's lecture on adaptive quadrature, using composite trapazoidal and regular simpson's rule.

References

[1] Victor Cumer. *The basics of Monte-Carlo integration*. Oct. 2020. URL: https://towardsdatascience.com/the-basics-of-monte-carlo-integration-5fe16b40482d.

[2] Adrian E. Feiguin. *Monte-Carlo error analysis*. Nov. 2009. URL: https://web.northeastern.edu/afeiguin/phys5870/phys5870/node71.html.

[3] Wojciech Jarosz. "Efficient Monte Carlo Methods for Light Transport in Scattering Media". PhD thesis. UC San Diego, Sept. 2008.

[4] *Monte Carlo integration*. Apr. 2022. URL: https://en.wikipedia.org/wiki/Monte_Carlo_integration#Example.

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[3] https://cs.dartmouth.edu/wjarosz/publications/dissertation/appendixA.pdf

[3] [4] [2] [5] [1]