Monte Carlo Integration

Mathematical and Numerical Methods
CDSC 603

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Little History

Introduction to Monte Carlo Method

Probability Background

The Monte Carlo Estimator

Expected Value and Convergence

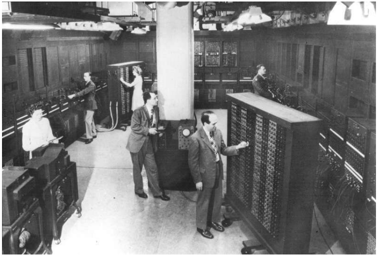
Multidimensional Integration

Variance Reduction

Importance Sampling

A Little History

- Ulam, recovering from an illness, was playing a lot of solitaire
- Tried to figure out probability of winning, and failed
- Thought about playing lots of hands and counting number of wins, but decided it would take years
- Asked Von Neumann if he could build a program to simulate many hands on ENIAC



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Introduction to Monte Carlo Method

- Often times, we can't solve integrals analytically and must resort to numerical methods. Among these include Monte Carlo integration. As you may remember, the integral of a function can be interpreted as *the area under a function's curve*.
- Monte Carlo integration works by evaluating a function at different random points between a and b, adding up the area of the rectangles and taking the average of the sum. As the number of points increases, the result approaches to the actual solution to the integral.
- Monte Carlo methods are numerical techniques which rely on random sampling to *approximate* their results. Monte Carlo integration applies this process to the numerical estimation of integrals.
- Monte Carlo integration is a technique for numerical integration using random numbers.

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Probability Background

In order to define Monte Carlo integration, we start by reviewing some basic ideas from probability.

Random Variables

A random variable X is a function that maps outcomes of a random process to numbers. A random variable can be either discrete (e.g., the roll of a six-sided die where a fixed set of outcomes is possible, $X = 1, 2, 3, 4, 5, 6$), or continuous (e.g., a person's height, which can take on real values $\mathbb{R}$). In computer graphics we more commonly deal with continuous random variables which take on values over ranges of continuous domains (e.g., the real numbers $\mathbb{R}$ or the sphere of directions Ω).

Cumulative Distributions and Density Functions

The cumulative distribution function, or CDF, of a random variable X is the probability that a value chosen from the variable's distribution is less than or equal to some thresold x:

$$cdf(x) = Pr\{X \leq x\} \tag{1}$$

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The corresponding probability density function, or PDF, is the derivative of the CDF:

$$pdf(x) = \frac{d}{dx} cdf(x) \tag{2}$$

CDFs are always monotonically increasing, which means that the PDF is always non-negative. An important relationship arises from the above two equations, which allows us to compute the probability that a random variable lies within an interval:

$$Pr\{a \leq X \leq b\} = \int_a^b pdf(x)dx \tag{3}$$

From this expression it is clear that the PDF must always integrate to one over the full extent of its domain.

Expected Values and Variance

The *expected value* or expectation of a random variable $Y = f(X)$ over a domain $\mu(x)$ is defined as

$$E[Y] = \int_{\mu} (x) f(x) pdf(x) d\mu(x) \tag{4}$$

while its *variance* is

$$\sigma^2[Y] = E[(Y - E(Y)^2] \tag{5}$$

where σ, the standard deviation, is the square root of the variance. From these definitions it is easy to show that for any constant a,

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$$E[aY] = aE[Y]\sigma^2[aY] = a^2\sigma^2[Y] \tag{6}$$

Furthermore, the expected value of a sum of random variables Y i is the sum of their expected values:

$$E\left[\sum_i Y_i\right] = \sum_i E[Y_i] \tag{7}$$

From these properties it is possible to derive a simpler expression for the variance:

$$\sigma^2[Y] = E[Y^2] - E[Y]^2 \tag{8}$$

Additionally, if the random variables are uncorrelated, a summation property also holds for *the variance*

$$\sigma^2\left[\sum_i Y_i\right] = \sum_i \sigma^2[Y_i] \tag{9}$$

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The Monte Carlo Estimator

The Basic Estimator. Monte Carlo integration uses random sampling of a function to numerically compute an estimate of its integral. Suppose that we want to integrate the one dimensional function $f(x)$ from a to b :

$$\int_a^b f(x)dx \tag{10}$$

We can approximate this integral by averaging samples of the function f at uniform random points within the interval. Given a set of N uniform random variables $X_i \in [a, b]$ with a corresponding PDF of $\frac{1}{(b-a)}$, the Monte Carlo estimator for computing F is

$$\langle F^N \rangle = (b-a)\frac{1}{N-1}\sum_{i=0}^{N} f(X_i), \tag{11}$$

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The random variable $X_i \in [a, b]$ can be constructed by warping a canonical random number uniformly distributed between zero and one, $\xi_i \in [0, 1]$:

$$X_i = a + \xi_i(b - a) \tag{12}$$

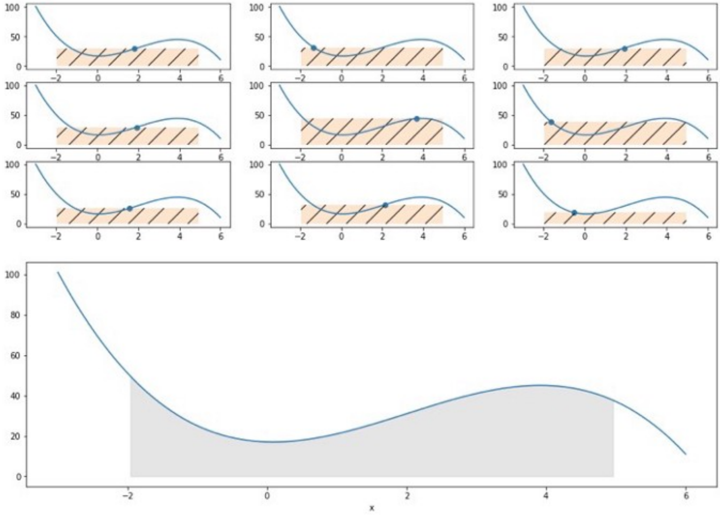
Using this construction, we can expand the estimator to:

$$\langle F^N \rangle = (b - a)\frac{1}{N}\sum_{i=0}^{N-1} f(a + \xi_i(b - a)), \tag{13}$$

Since F^N is a function of X_i , it is itself a random variable. We use this notation to clarify that $\langle F^N \rangle$ is an approximation of F using N samples.

Example 1

Integrals can be interpreted as the area below the function's curve.
Let's take the following function as an example:
$f(x) = -x^3 + 6x^2 - x + 17$ ... let $a = -2$ and $b = 5$



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Expected Value and Convergence

It is easy to show that the expected value of $\langle F^N \rangle$ is in fact F:

$$
\begin{aligned}
[\langle F^N \rangle] &= [(b-a)\frac{1}{N}\sum_{i=0}^{N-1} f(x_i)] \\
&= (b-a)\frac{1}{N}\sum_{i=0}^{N-1} E[f(x_i)], \\
&= (b-a)\frac{1}{N}\sum_{i=0}^{N-1} \int_a^b f(x)pdf(x)dx, \\
&= \frac{1}{N}\sum_{i=0}^{N-1} \int_a^b f(x)pdf(x)dx, \\
&= \int_a^b f(x)dx, \\
&= F
\end{aligned}
\tag{14}
$$

Furthermore, as we increase the number of samples N , the estimator F^N becomes a closer and closer approximation of F

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Furthermore, as we increase the number of samples N , the estimator F^N becomes a closer and closer approximation of F . Due to the Strong Law of Large Numbers, in the limit we can guarantee that we have the exact solution:

$$Pr\{\lim_{N\to\infty} \langle F^N \rangle = F\} = 1 \tag{15}$$

The Monte Carlo estimator converges in probability to F, the true value of the integral.

Another important result we get from the Monte Carlo estimator is the variance of the estimator: σ^2/N where σ is the standard deviation of the function values, and N is the number of samples X_i.

$$\sigma[\langle F^N \rangle] \propto \frac{1}{\sqrt{N}} \tag{16}$$

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Multidimensional Integration

Monte Carlo integration can be generalized to use random variables drawn from arbitrary PDFs and to compute multidimensional integrals, such as

$$F = \int_{\mu(x)} f(x) d\mu(x), \tag{17}$$

which can be modifed as ...

$$\langle F^N \rangle = \frac{1}{N} \sum_{i=0}^{N-1} \frac{f(X_i)}{pdf(X_i)} \tag{18}$$

It is similarly easy to show that this generalized estimator also has the correct expected value ..... $= F$ ...... (You do the math)

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Variance Reduction

Sources of Variance. In order to improve the quality of Monte Carlo integration we need to reduce variance. Since the samples in Monte Carlo integration are independent, the variance of $\langle F^N \rangle$ can be simplified to:

$$\begin{aligned}
\sigma^2[\langle F^N \rangle] &= \sigma^2[\frac{1}{N}\sum_{i=0}^{N-1}\frac{f(X_i)}{pdf(X_i)}] \\
&= \frac{1}{N^2}\sum_{i=0}^{N-1}\sigma^2[\frac{f(X_i)}{pdf(X_i)}] \\
&= \frac{1}{N^2}\sum_{i=0}^{N-1}\sigma^2[Y_i] \\
&= \frac{1}{N}\sigma^2[Y] \qquad (19)
\end{aligned}$$

and hence,

$$\sigma[\langle F^N \rangle] = \frac{1}{\sqrt{N}}\sigma[Y] \qquad (20)$$

Importance Sampling

The idea behind Importance Sampling is very simple: as the error of the Monte Carlo estimator is proportional to the standard deviation of $f(x)$ divided by the square root of the number of samples, we should find a cleverer method to chose X_i than the uniform law.

The Perfect Estimator : To demonstrate the effect of importance sampling, consider a PDF which is exactly proportional to the function being integrated, $pdf(x) = cf(x)$ for some normalization constant c. Since c is a constant, if we apply this PDF to the Monte Carlo estimator in Equation 18, each sample X_i would have the same value,

$$Y_i = \frac{f(X_i)}{pdf(X_i)} = \frac{f(X_i)}{cf(X_i)} = \frac{1}{c} \tag{21}$$

Since the PDF must integrate to one, it is easy to derive the value of c:

$$c = \frac{1}{\int f(x)dx} \tag{22}$$

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Notebook attached with Examples in Python and Exercise to practice

Thank You

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