Topic 10 The Law of Large Numbers Monte Carlo Integration

Outline

Simple Monte Carlo Integration

Importance Sampling

Monte Carlo methods is a collection of computational algorithms that use stochastic simulations to approximate solutions to questions that are very difficult to solve analytically.

This approach has seen widespread use in fields as diverse as statistical physics, astronomy, population genetics, protein chemistry, and finance.

Let $X_1, X_2, ...$ be independent random variables uniformly distributed on the interval [a, b] and write f_X for their common density.

Then, by the law of large numbers, for n large we have that

$$\overline{g(X)}_n = \frac{1}{n} \sum_{i=1}^n g(X_i) \approx Eg(X_1) = \int_a^b g(x) f_X(x) \ dx = \frac{1}{b-a} \int_a^b g(x) \ dx.$$

Thus,
$$\int_{a}^{b} g(x) dx \approx (b-a)\overline{g(X)}_{n}$$
.

Recall that in calculus, we defined the average of g to be

$$\frac{1}{b-a}\int_a^b g(x) dx.$$

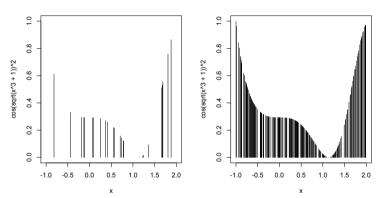
We can now interpret this integral as an expected value.

Thus, Monte Carlo integration leads to a procedure for estimating integrals.

- Simulate uniform random variables X_1, X_2, \dots, X_n on the interval [a, b],
- Evaluate $g(X_1), g(X_2), ..., g(X_n)$.
- Average this values and multiply by b a to estimate the integral.

Let $\cos^2(\sqrt{x^3+1})$ for $x \in [-1,2]$, to find $\int_{-2}^1 g(x) dx$. The three steps above become the following R code.

```
> x<-runif(250,-1,2)
> g<-cos(sqrt(x^3+1))^2
> 3*mean(g)
[1] 1.074919
```



Monte Carlo integration of $g(x) = \cos^2(\sqrt{x^3 + 1})$ on [-1, 2], we simulate n uniform random variables using runif (n, -1, 2) and then use R to compute $3*mean(\cos(\operatorname{sqrt}(x^3+1))^2)$. n = 25 (left) and n = 250 (right) are shown

With only a small change in the algorithm, we can also use this to evaluate multivariate integrals. For example, in three dimensions, the integral

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} \int_{a_3}^{b_3} g(x,y,z) \, dz \, dy \, dx \approx (b_1 - a_1)(b_2 - a_2)(b_3 - a_3) \frac{1}{n} \sum_{i=1}^n g(X_i, Y_i, Z_i).$$

where $X_i \sim U(a_1, b_1)$, $Y_i \sim U(a_2, b_2)$, and $Z_i \sim U(a_3, b_3)$

Example. To estimate

$$\int_{-2}^{2} \int_{1/2}^{1} \int_{0}^{1} \frac{e^{-x^{2}/2y}}{x^{2}z+1} dz dy dx$$

```
> x<-runif(250,-2,2);y<-runif(250,1/2,1);z<-runif(250)
```

- $> g < -exp(-x^2/(2*y))/(x^2*z+2)$
- > 4*0.5*1*mean(g)
- [1] 0.4550264

Monte Carlo integration uses the averages of a simulated random sample and consequently, its value is itself random. To obtain a sense of the distribution of the approximations to the integral

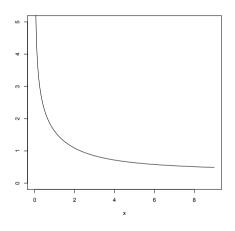
$$\int_0^8 \frac{1 + e^{-x/2}}{\sqrt[3]{x}} \ dx,$$

we perform 1000 simulations using 250 uniform random variables. The command Ig<-rep(0,1000) creates a vector of 1000 zeros. This is added so that R has a place ahead of the simulations to store the results.

```
> Ig<-rep(0,1000)
> for (i in 1:1000){x<-runif(250,0,8);Ig[i]<-8*mean((1+exp(-x/2))/x^(1/3))}
> mean(Ig)
[1] 8.120468
> sd(Ig)
[1] 0.4715746
```

To reduce the standard deviation, we can

- Increase the size of the simulation.
 - An increase from 250 to 1000
 decreases the variance by a factor of
 4 and thus the standard deviation by
 a factor of 2.
- Concentrate the values of x where the function g changes rapidly.
 - Such a strategy is called importance sampling.



The graph of g(x)

Goal. Reduce the standard deviation in the approximation of the integral

$$\int_{a}^{b} g(x) dx$$

Write $g(x) = w(x)f_X(x)$ where

- $f_X(x)$ is a density function that captures the change in g(x) and has an easy to determine distribution function $F_X(x)$.
 - f_X is called the importance sampling function or the proposal density.
 - w is called the importance sampling weight.

Now, simulate X_1, X_2, \dots, X_n independent random variables with common density f_X . Then by the law of large numbers.

$$\frac{1}{n} \sum_{i=1}^{n} w(X_i) \approx Ew(X_1) = \int_{a}^{b} w(x) f_X(x) \ dx = \int_{a}^{b} g(x) \ dx.$$

$$\int_0^8 \frac{1 + e^{-x/2}}{\sqrt[3]{x}} \ dx = \int_0^8 (1 + e^{-x/2}) \frac{1}{\sqrt[3]{x}} \ dx$$

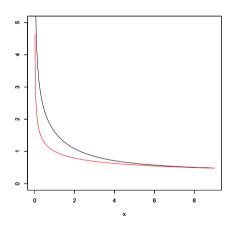
The distribution function

$$F_x(x) = c \int_0^x \frac{1}{\sqrt[3]{t}} dt = \frac{3c}{2} t^{2/3} \Big|_0^x = \frac{3c}{2} x^{2/3}$$

Now,
$$1 = F_X(8) = \frac{3c}{2}8^{2/3} = \frac{3c}{2}4 = 6c$$
.

So,
$$c = 1/6$$
 and $f_X(x) = \frac{1}{6\sqrt[3]{x}}$ is a density

and distribution function
$$F_X(x) = \frac{1}{4}x^{2/3}$$
 on [0, 8].



The graph of g(x) (black) and the proposal density $f_X(x)$ (red)

$$\int_{a}^{b} g(x) \ dx = \int_{a}^{b} w(x) f_{X}(x) \ dx$$
$$\int_{0}^{8} \frac{1 + e^{-x/2}}{\sqrt[3]{x}} \ dx = \int_{0}^{8} 6(1 + e^{-x/2}) \frac{1}{6} \frac{1}{\sqrt[3]{x}} \ dx$$

So,

the density
$$f_X(x) = \frac{1}{6\sqrt[3]{x}}$$
 and the weight function $w(x) = 6(1 + e^{x/2})$.

To simulate the X_i we use the probability transform.

$$u = F_x(x) = \frac{1}{4}x^{2/3}$$
. Thus, $x = (4u)^{3/2}$.

For the probability transform in R we enter u < runif(250); $x < -(4*u)^3/2$. Thus, for 1000 importance sampling approximations, we find

```
> ISg<-rep(0,1000)
> for (i in 1:1000){u<-runif(250);x<-(4*u)^(3/2);ISg[i]<-mean(6*(1+exp(-x/2)))}
> mean(ISg)
[1] 8.132918
> sd(ISg)
[1] 0.1164385
```

Compare this with simple Monte Carlo.

```
> sd(Ig)
[1] 0.4715746
```

The standard deviation is reduced by a factor of \sim 4 and thus, we would need to increase the number of simulations by a factor of \sim 16 for simple Monte Carlo to meet the same standard deviation.