Biostatistics 615/815 Lecture 16: Monte-carlo methods Importance sampling

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Annoucements

Grading

- Midterm will be given by Thursday
- All the other homeworks will be given by next Tuesday

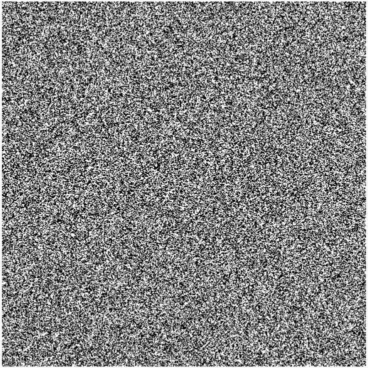
815 Update

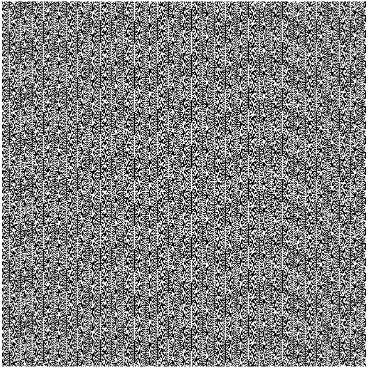
- Send a brief progress update on the project
- Schedule meeting with instructor if needed

Recap : Pseudo-random numbers using rand()

```
#include <iostream>
#include <cstdlib>
int main(int argc, char** argv) {
  int n = (argc > 1) ? atoi(argv[1]) : 1;
  int seed = (argc > 2 ) ? atoi(argv[2]) : 0;

  srand(seed); // set seed -- same seed, same pseudo-random numbers

  for(int i=0; i < n; ++i) {
    std::cout << (double)rand()/RAND_MAX << std::endl;
    // generate value between 0 and 1
  }

  return 0;
}
```

Recap : Good vs. bad random numbers





- Images using true random numbers from `random.org` vs. `rand()` function in PHP
- Visible patterns suggest that `rand()` gives predictable sequence of pseudo-random numbers

Recap : Generating uniform random numbers in C++

```
#include <iostream>
#include <boost/random/uniform_int.hpp>
#include <boost/random/uniform_real.hpp>
#include <boost/random/variate_generator.hpp>
#include <boost/random/mersenne_twister.hpp>
int main(int argc, char** argv) {
  typedef boost::mt19937 prgType; // Mersenne-twister : a widely used
  prgType rng;       //    lightweight pseudo-random-number-generator
  boost::uniform_int<> six(1,6);  // uniform distribution from 1 to 6
  boost::variate_generator<prgType&, boost::uniform_int<> > die(rng,six);
  // die maps random numbers from rng to uniform distribution 1..6

  int x = die();     // generate a random integer between 1 and 6
  std::cout << "Rolled die : " << x << std::endl;

  boost::uniform_real<> uni_dist(0,1);
  boost::variate_generator<prgType&, boost::uniform_real<> > uni(rng,uni_dist);
  double y = uni();  // generate a random number between 0 and 1
  std::cout << "Uniform real : " << y << std::endl;
  return 0;
}
```

Today

Sampling from complex distributions

- Monte-Carlo Methods
- Importance Sampling

Monte-Carlo Methods

Informal definition

- Approximation by random sampling
- Randomized algorithms to solve deterministic problems approximately.

An example problem

Calculating

$$I = \int_0^1 f(x)\,dx$$

where $f(x)$ is a complex function with $0 \leq f(x) \leq 1$
The problem is equivalent to computing $E[f(u)]$ where $u \sim U(0,1)$.

The crude Monte-Carlo method

Algorithm

- Generate $u_1, u_2, \cdots, u_B$ uniformly from $U(0,1)$.
- Take their average to estimate θ

$$\hat{\theta} = \frac{1}{B} \sum_{i=1}^{B} f(u_i)$$

The crude Monte-Carlo method

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Desirable properties of Monte-Carlo methods

- Consistency : Estimates converges to true answer as B increases
- Unbiasedness : $E[\hat{\theta}] = \theta$
- Minimal Variance

Analysis of crude Monte-Carlo method

Bias

$$E[\hat{\theta}] = \frac{1}{B}\sum_{i=1}^{B} E[f(u_i)] = \frac{1}{B}\sum_{i=1}^{B} \theta = \theta$$

Analysis of crude Monte-Carlo method

Bias

$$E[\hat{\theta}] = \frac{1}{B}\sum_{i=1}^{B} E[f(u_i)] = \frac{1}{B}\sum_{i=1}^{B} \theta = \theta$$

Variance

$$\begin{aligned}\sigma^2 &= \frac{1}{B}\int_0^1 (f(u)-\theta)^2\,du \\ &= \frac{1}{B}E[f(u)^2] - \frac{\theta^2}{B}\end{aligned}$$

Analysis of crude Monte-Carlo method

Bias

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Variance

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Consistency

$$\lim_{B\to\infty} \hat{\theta} = \theta$$

Accept-reject (or hit-and-miss) Monte Carlo method

Algorithm

1. Define a rectangle R between $(0,0)$ and $(1,1)$
2. Set $h = 0$ (hit), $m = 0$ (miss).
3. Sample a random point $(x, y) \in R$.
4. If $y < f(x)$, then increase h. Otherwise, increase m
5. Repeat step 3 and 4 for B times
6. $\hat{\theta} = \frac{h}{h+m}$.

Analysis of accept-reject Monte Carlo method

Bias

Let u_i, v_i follow $U(0,1)$.

$$E[\hat{\theta}] = E\left[\frac{h}{h+m}\right] = \theta$$

Analysis of accept-reject Monte Carlo method

Bias

Let u_i, v_i follow $U(0,1)$.

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Variance

$$\sigma^2 = \frac{\theta(1-\theta)}{B}$$

Which method is better?

$$\begin{aligned}
\sigma^2_{AR} - \sigma^2_{crude} &= \frac{\theta(1-\theta)}{B} - \frac{1}{B}E[f(u)^2] + \frac{\theta^2}{B} \\
&= \frac{\theta - E[f(u)]^2}{B} \\
&= \frac{1}{B}\int_0^1 f(u)(1-f(u))\,du \geq 0
\end{aligned}$$

The crude Monte-Carlo method has less variance then accept-rejection method

Revisiting The Crude Monte Carlo

$$\begin{aligned}\theta &= E[f(u)] = \int_0^1 f(u)\,du \\ \hat{\theta} &= \frac{1}{B}\sum_{i=1}^{B} f(u_i)\end{aligned}$$

More generally, when x has pdf $p(x)$, if x_i is random variable following $p(x)$,

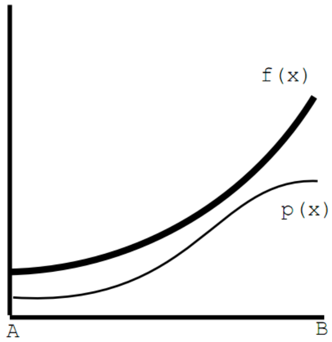
$$\begin{aligned}\theta &= E_p[f(x)] = \int f(x)p(x)\,dx \\ \hat{\theta} &= \frac{1}{B}\sum_{i=1}^{B} f(x_i)\end{aligned}$$

Importance sampling

Let x_i be random variable, and let $p(x)$ be an arbitrary function.

$$\begin{aligned}\theta &= E_u[f(x)] \int f(x)\,dx = \int \frac{f(x)}{p(x)} p(x)\,dx = E_p\left[\frac{f(x)}{g(x)}\right] \\ \hat{\theta} &= \frac{1}{B}\sum_{i=1}^{B} \frac{f(x_i)}{p(x_i)}\end{aligned}$$

Key Idea



- When $f(x)$ is not uniform, variance of $\hat{\theta}$ may be large.
- The idea is to pretend sampling from (almost) uniform distribution.

Importance sampling reduces the variance of θ

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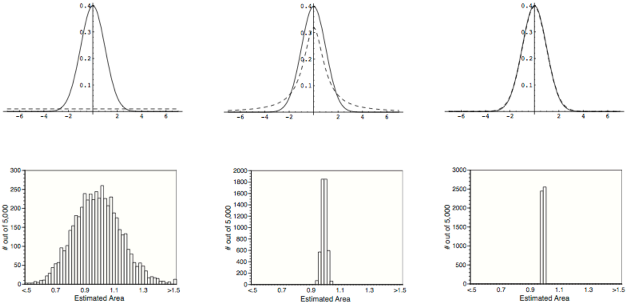

(a) Uniform (b) t_1 Dist. (c) t_30 Dist.

Figure 1: Three different importance sampling functions (dotted lines) used to integrate the standard normal density (solid line) from -50 to 50. Top panels are the density curves and bottom panels are histograms of 5,000 Monte Carlo estimates of the area (which is exactly 1) using $n = 1,000$.

More on rejection sampling

Framework for random sampling with inversion CDF

- Draw $u \sim U(0,1)$.
- Set $x = F^{-1}(u)$ for a CDF F.
- Then x is a random variable such that $x \sim F$

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Framework for random sampling with inversion CDF

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Rejection sampling

1. Sample (x, u) from rectagle coveraging $\min f(x) \leq u \leq \max f(x)$.
2. Accept x if $u \leq f(x)$.
3. Otherwise, reject and repeat step 1 and 2 until accept
4. Repeat step 1-3 to obtain multiple random variable following $x \sim F$

Summary

- Crude Monte Carlo method : Sampling from uniform distribution for estimating θ.
- Rejection sampling : Used for calculating θ, or generating random samples
- Importance sampling : Reweight the probability distribution to reduce the variance in the estimation