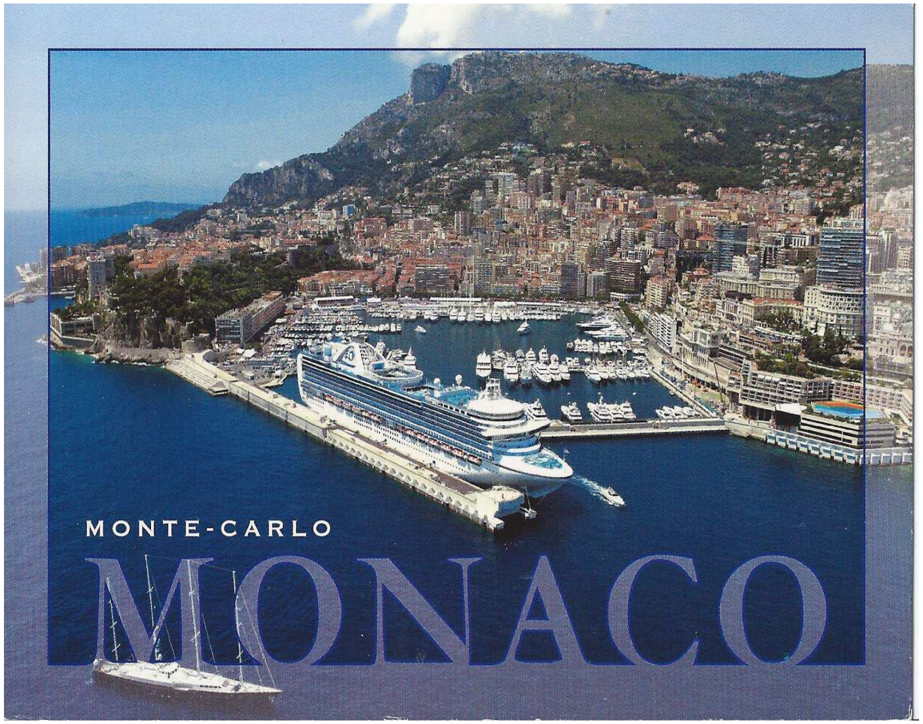
Introduction to Monte Carlo Methods

STAT 525

8/28/18

What is Monte Carlo ?

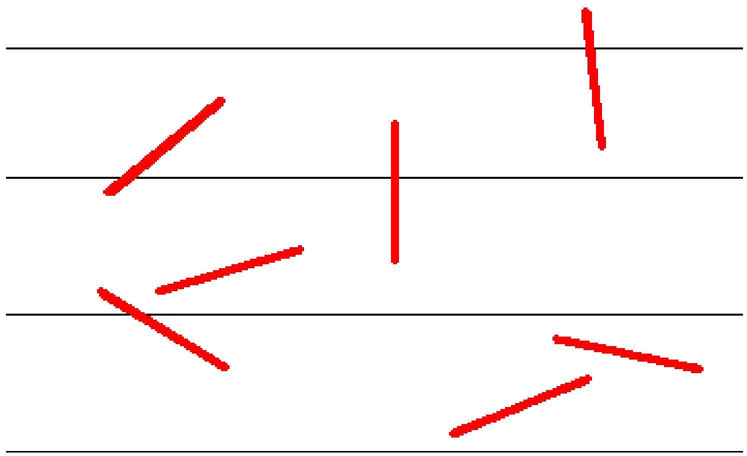
- Monte Carlo methods are a class of computational algorithms that rely on repeated random sampling to compute their results (Wikipedia).
- It is named after the famous European gambling center in Monaco.



- Monte Carlo methods are used to estimate probabilistic features of models that cannot be computed analytically.
- Examples:
  - Simulate traffic patterns
  - Simulate behavior of gas molecures
  - Blackjack (also known as Twenty-one).

History

- The basic idea of Monte Carlo computation can be traced back to "Buffon's needle", introduced by Buffon in 1777, which can be used to estimate π.



- Let N be the total number of times that the needle is randomly dropped on the table, and C be the number of times that it crosses a line.

- Keep dropping the needle, eventually $\frac{2N}{C} \to \pi$.

- Why? It is not hard to show, with a little bit of calculus, that

$$\text{P(needle crosses a line)} = \frac{2}{\pi}.$$

  As N increases, $\frac{C}{N} \to \frac{2}{\pi}$.

- Applet available at *http://www.angelfire.com/wa/hurben/buff.html*

- The systematic development of Monte Carlo methods started from about 1944. In the past several decades, many new Monte Carlo techniques have been developed, such as sequential Monte Carlo, Markov chain Monte Carlo (MCMC).

- Monte Carlo methods have become an important topic in scientific computing and are now routinely used in many diverse fields, such as computational biology, engineering, economics, finance, physics and statistics.

AlphaGo versus Lee Sedol

- AlphaGo: Developed by Google DeepMind to play Go.
- In March 2016, it beat Lee Sedol in a 5-game match.

  It was chosen by Science as one of the Breakthrough of the Year.

- AlphaGo's algorithm uses a **Monte Carlo** tree search to find its moves based on knowledge previously "learned" by machine learning (wikipedia).

Basic problems of Monte Carlo

- There are two basic problems of Monte Carlo. One is to draw random samples from a probability distribution function $\pi(\mathbf{x})$; the other is to estimate the integral

$$\mu = \int h(\mathbf{x})\pi(\mathbf{x})d\mathbf{x} = E_\pi\{h(\mathbf{X})\}.$$

- Many scientific and statistical problems involve integration over probability distributions, e.g., Bayes estimators and p-values.

Naive Monte Carlo

- Want to estimate

$$\mu = E_\pi\{h(\mathbf{X})\} = \int h(\mathbf{x})\pi(\mathbf{x})d\mathbf{x}.$$

- Naive Monte Carlo
  - Draw i.i.d. samples $\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}$ from $\pi(\mathbf{x})$.
  - Estimate μ by

$$\hat{\mu}_m = \frac{1}{m}[h(\mathbf{x}^{(1)}) + \cdots + h(\mathbf{x}^{(m)})].$$

- By Strong Law of Large Numbers,

$$\hat{\mu}_m \longrightarrow \mu \qquad \text{a.s.}$$

  and its convergence rate can be assessed by the Central Limit Theorem:

$$\sqrt{m}(\hat{\mu}_m - \mu) \Longrightarrow N(0, \sigma^2),$$

  where $\sigma^2 = Var\{h(\mathbf{X})\}$. Hence, the error rate is of order $O(m^{-1/2})$.

- Deterministic numerical methods do not scale well when the dimensionality of $\mathbf{x}$ increases, while the order of accuracy for the Monte Carlo approach is not affected by the dimensionality of $\mathbf{x}$. This advantage underlies the potential role of the Monte Carlo methodology in science and statistics.

Generating Random Variables

- Mechanical devices (e.g., coin-tossing, card shuffling, electronic noise, . . .)
- Generate *pseudo-random* numbers. A sequence of *pseudo-random* numbers (U_i) is a deterministic sequence of numbers in [0,1] having the same relevant statistical properties as a sequence of random numbers.
- Congruential generator:

$$X_i = aX_{i-1} \text{ mod } M.$$

For example, $a = 23$, $M = 10^8 + 1$. Then $U_i = \frac{X_i}{M} \in [0, 1]$.

Generate Non-Uniform Random Variables

The Inversion method

- Lemma: Suppose $U \sim$ Unif [0,1] and F is a one-dimensional cumulative distribution function (cdf). Then

$$X = F^{-1}(U)$$

has the distribution F. Here we define

$$F^{-1}(u) = \inf\{x : F(x) \geq u\}.$$

- Example 1. Exponential random variables with pdf
  $f(t) = \lambda e^{-\lambda t}$, $t > 0$.

- Example 2. Cauchy random variables with pdf $f(t) = \frac{1}{\pi(1+t^2)}$, $-\infty < t < \infty$.

Special Methods

- Standard normal random variables:
  - Generate U_1 and U_2 from Unif [0,1].
  - Then

$$\begin{aligned} X &= \sqrt{-2\log(U_1)}\cos(2\pi U_2) \\ Y &= \sqrt{-2\log(U_1)}\sin(2\pi U_2) \end{aligned}$$

    are two independent samples from $N(0,1)$.

- A Beta random variable can be constructed as the ratio $X_1/(X_1+X_2)$, where X_1 and X_2 are independent Gamma random variables.

References

- Sections 1.1 and 2.1 of Jun Liu's *Monte Carlo Strategies in Scientific Computing*.