Chapter 3 - Monte Carlo Methods

Introduction to Monte Carlo Methods.

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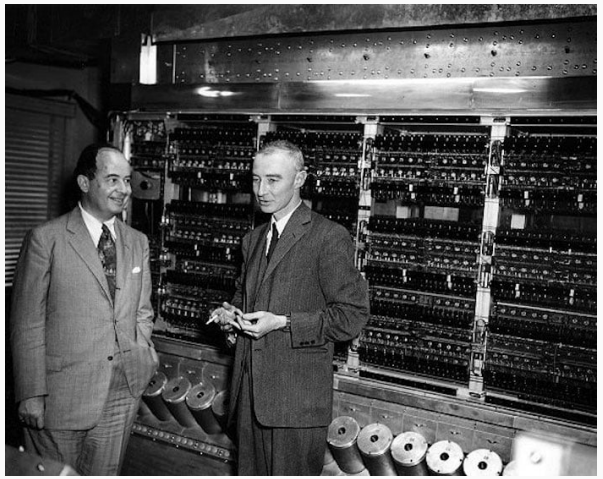
History of the Monte Carlo Method

- The Monte Carlo method was developed in the 1940s during research for the Manhattan Project.
- Mathematician Stanislaw Ulam conceived the idea while recovering from an illness, inspired by thinking about solitaire.
- He wondered: *"What is the expected number of winning hands in a game of solitaire?"*
- This question led to the use of repeated random sampling to estimate expectations — the foundation of Monte Carlo simulation.

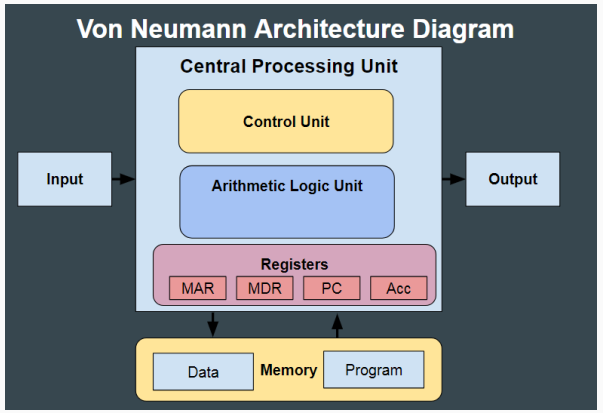
Stanislaw Ulam (1909–1984)

Early Development and Implementation

- Ulam proposed using random sampling to solve complex problems in neutron diffusion.
- John von Neumann and colleagues formalized the method and implemented it on the ENIAC computer, one of the earliest electronic computers.
- The name *"Monte Carlo"* was inspired by the frequent trips of Ulam's uncle to the casino in Monte Carlo, Monaco.



ENIAC - John von Neumann and Oppenheimer



Von Neumann architecture

Introduction to Monte Carlo Methods

- Monte Carlo methods are a general class of computational algorithms that generate random scenarios to obtain numerical results.
- These methods are widely used in statistical physics, computational chemistry, statistical inference, genetics, and finance.
- The Metropolis algorithm, a key Monte Carlo technique, was named one of the top algorithms of the 20th century by a committee of mathematicians, computer scientists, and physicists.
- The increasing availability of computational power has greatly expanded the use of Monte Carlo simulations.
- Monte Carlo methods can be used to solve a variety of mathematical problems. **In its most basic form, we use it as a numerical integration method** for integrals with no explicit solution. In this course we will also explore other uses of Monte Carlo methods.

Motivation: Particle in a Random Medium

- Consider a particle $(X_t)_{t=1,2,\dots}$ moving in space $\Omega = \mathbb{R}^d$ according to a stochastic model (e.g., random walk, diffusion, or Markov chain). Randomness may arise from the environment ("medium") or from the particle's motion.
- **Absorption rule:** At each time step t, the particle can be absorbed with probability $1 - G(X_t)$, where $G : \Omega \to [0, 1]$ is the **survival weight** at location X_t.
  - $G(x) \approx 1$: safe location (low absorption risk)
  - $G(x) \approx 0$: high absorption risk (almost surely absorbed)
- The survival probability up to time T is

$$\mathbb{P}(\text{not absorbed at time } T) = \mathbb{E}\Big[\prod_{t=1}^{T} G(X_t)\Big].$$

Multiple Particles in a Random Medium

- Suppose we have n independent particles, each evolving over T time steps according to the stochastic model.
- Let $X_{i,t}$ denote the position of particle i at time t, for $i = 1, \ldots, n$ and $t = 1, \ldots, T$.
- Let $G(X_{i,t})$ denote the survival weight at that position.
- The joint survival probability for all particles is

$$\mathbb{P}(\text{all particles survive up to } T) = \mathbb{E}\Big[\prod_{i=1}^{n}\prod_{t=1}^{T} G(X_{i,t})\Big].$$

- For continuous positions, this is a $(n \cdot T)$-dimensional integral:

$$\mathbb{E}\Big[\prod_{i=1}^{n}\prod_{t=1}^{T} G(X_{i,t})\Big] = \int \cdots \int \prod_{i=1}^{n}\prod_{t=1}^{T} G(x_{i,t})\, p(x_{1,1}, \ldots, x_{n,T})\, dx_{1,1} \cdots dx_{n,T}$$

where $p(\cdot)$ is the joint density of all particle positions.

Computing Expected Values

Let $X = (X_1, X_2, \ldots, X_d)$ be a random vector with joint density $f(x_1, x_2, \ldots, x_d)$ and $g : \mathbb{R}^d \to \mathbb{R}$. We want to compute:

$$Eg(X) = \int_{\mathbb{R}^d} g(x) f(x) dx$$

If the integral on the right hand side cannot be solved explicitly, we are only left with numerical methods to get an approximated value of that integral.

To simplify the presentation we will assume next that we are in the one-dimensional case ($d = 1$) but most results apply also in the multidimensional case.

The Law of Large Numbers (LLN)

Theoretical Foundation of Monte Carlo Methods

The Monte Carlo method relies on the **Law of Large Numbers (LLN)**, which ensures that empirical averages converge to their expected values as the sample size grows.

Theorem (Strong Law of Large Numbers): Let $(X_i)_{i=1}^{\infty}$ be a sequence of independent and identically distributed (i.i.d.) random variables with

$$\mathbb{E}[X_i] = \mu, \quad \mathrm{Var}(X_i) = \sigma^2 < \infty$$

Then, as $n \to \infty$,

$$\overline{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i \xrightarrow{\text{a.s.}} \mu$$

i.e., the sample mean converges almost surely to the true mean.

Consequences of the Law of Large Numbers

- Suppose $X_1, X_2, \ldots, X_n$ is a simulated random sample from a random variable X with probability density function $f(x)$.
- Then, by the Law of Large Numbers,

$$\frac{1}{n}\sum_{j=1}^{n} g(X_j) \approx \mathbb{E}[g(X)] = \int_{\mathbb{R}} g(x)\, f(x)\, dx$$

  provided n is large.
- In particular, if $U_1, U_2, \ldots, U_n$ are independent random variables uniformly distributed on $[0, 1]$, then

$$\frac{1}{n}\sum_{j=1}^{n} g(U_j) \approx \mathbb{E}[g(U)] = \int_{0}^{1} g(x)\, dx$$

Monte Carlo Integration Example

Example: Compute by Monte Carlo integration $\int_0^\pi \sin x dx$.

Solution: Make the change of variable $y = \frac{1}{\pi}x$, then:

$$\int_0^\pi \sin x dx = \pi \int_0^1 \sin(\pi y) dy$$

Algorithm 1 Monte Carlo Estimation of $\pi \int_0^1 \sin(\pi x)\, dx$

1: **Input:** Number of samples n
2: Generate independent random variables $U_1, U_2, \ldots, U_n \sim \text{Uniform}(0, 1)$
3: Compute the empirical mean:

$$\widehat{I}_n = \pi \frac{1}{n} \sum_{j=1}^{n} \sin(\pi U_j)$$

4: **Output:** Monte Carlo estimate $\widehat{I}_n$ of the integral

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Monte Carlo Integration Example

Example: Compute by Monte Carlo integration

$$\int_0^1 \int_0^1 \sqrt{x+y} e^{xy} \, dx dy$$

Algorithm 2 Monte Carlo Estimator for $\mathbb{E}\left[\sqrt{U+V}\, e^{UV}\right]$

1: **Input:** Number of samples n

2: **Generate** $U_1, U_2, \ldots, U_n \sim \text{Uniform}(0,1)$

3: **Generate** $V_1, V_2, \ldots, V_n \sim \text{Uniform}(0,1)$

4: **Compute:**

$$\text{Empirical Mean} = \frac{1}{n} \sum_{j=1}^{n} \sqrt{U_j + V_j}\, e^{U_j V_j}$$

5: **Output:** Estimated value of $\mathbb{E}\left[\sqrt{U+V}\, e^{UV}\right]$

Homework

1. Compute using a Monte Carlo method $E\left[Z^{2/3}(|Z|+1)\right]$ where Z is a standard normal random variable.
2. Compute by Monte Carlo integration

$$\int_0^1 \int_0^2 (x+2y)\ln(3x+2y+1)dxdy$$

Hint: First make a change of variable so that the region of integration is the square $[0,1]\times[0,1]$