

Monte Carlo Methods: Early History and The Basics

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Outline of the Talk

Early History of Probability Theory and Monte Carlo Methods

Early History of Probability Theory

The Stars Align at Los Alamos

The Problems

The People

The Technology

Monte Carlo Methods

The Birth

General Concepts of the Monte Carlo Method

Future Work

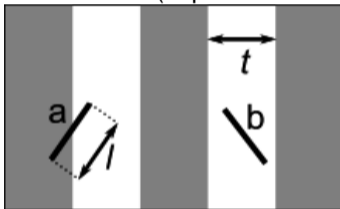
References

Early History of Probability Theory

- ▶ Probability was first used to understand games of chance
 1. Antoine Gombaud, chevalier de Méré, a French nobleman called on Blaise Pascal and Pierre de Fermat were called on to resolve a dispute
 2. Correspondence between Pascal and Fermat led to Huygens writing a text on “Probability”
 3. Jacob Bernoulli, Abraham de Moivre, and Pierre-Simon, marquis de Laplace, led development of modern “Probability”
 4. 1812: Laplace, *Théorie Analytique des Probabilités*

Early History of Monte Carlo: Before Los Alamos

- ▶ Buffon Needle Problem: Early Monte Carlo (experimental mathematics)



1. Problem was first stated in 1777 by Georges-Louis Leclerc, comte de Buffon
 2. Involves dropping a needle on a lined surface and can be used to estimate π
 3. Note: Union Capt. Fox did this while in a CSA prison camp, and produced good results that later turned out to be “fudged”
- ▶ In the 1930's, Fermi used sampling methods to estimate quantities involved in controlled fission

The Stars Align at Los Alamos

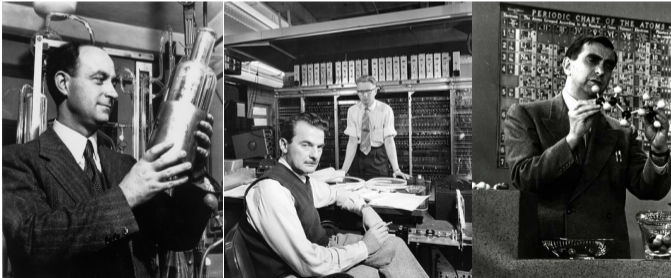
- ▶ Los Alamos brought together many interesting factors to give birth to modern Monte Carlo algorithms
 1. The Problems: Simulation of neutron histories (neutronics), hydrodynamics, thermonuclear detonation
 2. The People: Enrico Fermi, Stan Ulam, John von Neumann, Nick Metropolis, Edward Teller, ...
 3. The Technology: Massive human computers using hand calculators, the Fermiac, access to early digital computers
- ▶ The Name: Ulam's uncle would borrow money from the family by saying that "I just have to go to Monte Carlo"

The Problems

- ▶ Simulation of neutron histories (neutronics)
 1. Given neutron positions/momenta, geometry
 2. Compute flux, criticality, fission yield
- ▶ Hydrodynamics due to nuclear implosion
- ▶ Simulation of thermonuclear reactions: ignition, overall yield
 1. All these problems were more easily solved using Monte Carlo/Lagrangian methods
 2. Geometry is problematic for deterministic methods but not for MC

The People

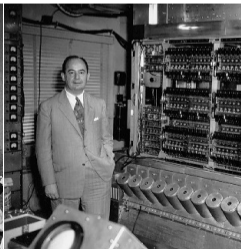
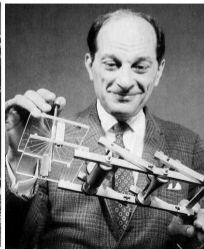
- ▶ Los Alamos brought together many interesting people to work on the fission problem:
- ▶ The Physicists
 1. Enrico Fermi: experimental Nuclear Physics and computational approaches
 2. Nick Metropolis: one of the first “computer programmers” for these problems
 3. Edward Teller: more interested in the “super”



The People

► The Mathematicians

1. Robert Richtmyer: ran the numerical analysis activities at Los Alamos
2. Stanislaw (Stan) Ulam: became interested in using “statistical sampling” for many problems
3. John von Neumann: devised Monte Carlo algorithms and helped develop digital computers



The Technology

- ▶ Simulation via computation was necessary to make progress at Los Alamos
- ▶ Many different computational techniques were in used
 1. Traditional digital computation: hand calculators used by efficient technicians
 2. Analog computers including the Fermiac (picture to follow)
 3. Shortly after the war, access to digital computers: ENIAC at Penn/Army Ballistics Research Laboratory (BRL)
 4. Continued development and acquisition of digital computers by Metropolis including the MANIAC

An Analog Monte Carlo Computer: The Fermiac

- ▶ Neutronics required simulating exponentially distributed flights based on material cross-sections
- ▶ Many neutron histories are required to get statistics
- ▶ Fermiac allows simulation of exponential flights inputting the cross-section manually
- ▶ Fermiac is used on a large piece of paper with the geometry drawn for neutronics simulations
- ▶ Fermiac allows an efficient graphical simulation of neutronics
- ▶ Parallelism is achievable with the Fermiac

An Analog Monte Carlo Computer: The Fermiac

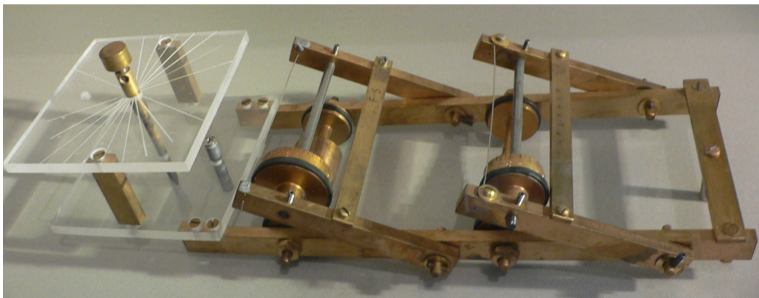


Figure: Enrico Fermi's Fermiac at the Bradbury Museum in Los Alamos

An Analog Monte Carlo Computer: The Fermiac

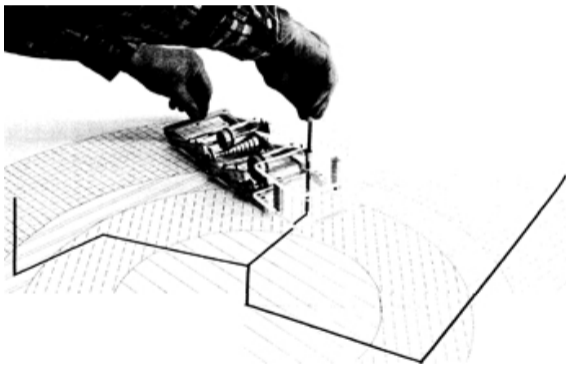


Figure: The Fermiac in Action

An Early Digital Computer: The ENIAC

- ▶ ENIAC: Electronic Numerical Integrator And Computer
- ▶ Funded by US Army with contract signed on June 5, 1943
- ▶ Built in secret by the University of Pennsylvania's Moore School of Electrical Engineering
- ▶ Completed February 14, 1946 in Philadelphia and used until November 9, 1946
- ▶ Moved (with upgrade) to Aberdeen Proving Grounds and began operations July 29, 1947
- ▶ Remained in continuous operation at the Army BRL until 1955

An Early Digital Computer: The ENIAC

- ▶ ENIAC is a completely programmable computer using first a plug panel
- ▶ ENIAC first contained (military rejects!)
 1. 17,468 vacuum tubes
 2. 7,200 crystal diodes
 3. 1,500 relays, 70,000 resistors
 4. 10,000 capacitors
 5. about 5 million hand-soldered joints
- ▶ Clock was 5KHz
- ▶ Ended up with a 100-word core memory
- ▶ Metropolis would go to BRL to work on the “Los Alamos” problem on the ENIAC

An Early Digital Computer: The ENIAC



An Early Digital Computer: The ENIAC

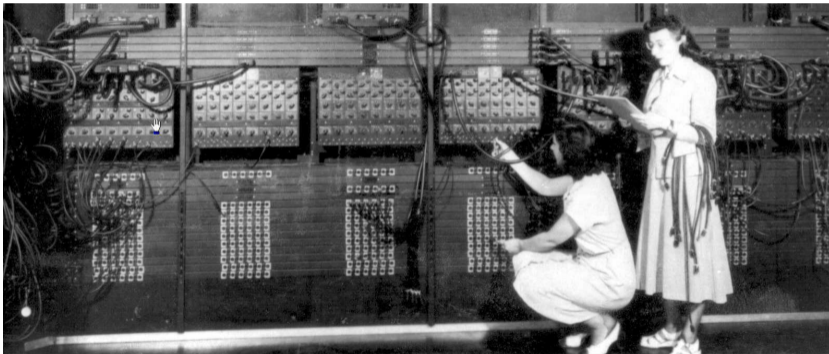


Figure: Programming the ENIAC

An Early Digital Computer: The ENIAC



The Birth of Monte Carlo Methods

- ▶ After the was digital computer was perfect for “statistical sampling”
 1. Individual samples were often very simple to program
 2. Small memory was not a big constraint for these methods
 3. A much better use for digital vs. human computers
- ▶ Early Monte Carlo Meetings
 1. 1952, Los Angeles: RAND Corp., National Bureau of Standards (NBS now NIST), Oak Ridge
 2. 1954, Gainesville, FL: University of Florida Statistical Lab

Integration: The Classic Monte Carlo Application

1. Consider computing $I = \int_0^1 f(x) dx$
2. Conventional quadrature methods:

$$I \approx \sum_{i=1}^N w_i f(x_i)$$

- ▶ *Rectangle*: $w_i = \frac{1}{N}$, $x_i = \frac{i}{N}$
- ▶ *Trapezoidal*: $w_i = \frac{2}{N}$, $w_1 = w_N = \frac{1}{N}$, $x_i = \frac{i}{N}$

3. Monte Carlo method has two parts to estimate a numerical quantity of interest, I

- ▶ The random process/variable: $x_i \sim U[0, 1]$ i.i.d.
- ▶ The score: $f(x_i)$
- ▶ One averages and uses a confidence interval for an error bound

$$\bar{I} = \frac{1}{N} \sum_{i=1}^N f(x_i), \quad \text{var}(I) = \frac{1}{N-1} \sum_{i=1}^N (f(x_i) - \bar{I})^2 = \frac{1}{N-1} \left[\sum_{i=1}^N f(x_i)^2 - N\bar{I}^2 \right],$$

$$\text{var}(\bar{I}) = \frac{\text{var}(I)}{N}, \quad I \in \bar{I} \pm k \times \sqrt{\text{var}(\bar{I})}$$

Other Early Monte Carlo Applications

- ▶ Numerical linear algebra based on sums: $S = \sum_{i=1}^N a_i$
 1. Define $p_i \geq 0$ as the probability of choosing index i , with $\sum_{i=1}^M p_i = 1$, and $p_i > 0$ whenever $a_i \neq 0$
 2. Then a_i/p_i with index i chosen with $\{p_i\}$ is an unbiased estimate of S , as

$$E[a_i/p_i] = \sum_{i=1}^M \left(\frac{a_i}{p_i}\right) p_i = S$$
- ▶ Can be used to solve linear systems of the form $x = Hx + b$
- ▶ Consider the linear system: $x = Hx + b$, if $\|H\| = \mathbb{H} < 1$, then the following iterative method converges:

$$x^{n+1} := Hx^n + b, \quad x^0 = 0,$$

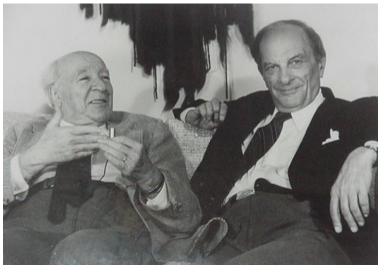
and in particular we have $x^k = \sum_{i=0}^{k-1} H^i b$, and similarly the Neumann series converges:

$$N = \sum_{i=0}^{\infty} H^i = (I - H)^{-1}, \quad \|N\| = \sum_{i=0}^{\infty} \|H^i\| \leq \sum_{i=0}^{\infty} \mathbb{H}^i = \frac{1}{1 - \mathbb{H}}$$

- ▶ Formally, the solution is $x = (I - H)^{-1} b$

Other Early Monte Carlo Applications

- ▶ Methods for partial differential and integral equations
 1. Integral equation methods are similar in construction to the linear system methods
 2. PDEs can be solved by using the Feynman-Kac formula
 3. Note Kac and Ulam both were trained in Lwów



Monte Carlo Methods: Numerical Experimental that Use Random Numbers

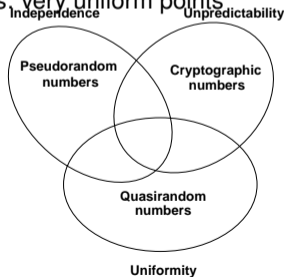
- ▶ A Monte Carlo method is any process that consumes random numbers
- 1. Each calculation is a numerical experiment
 - ▶ Subject to known and unknown sources of error
 - ▶ Should be reproducible by peers
 - ▶ Should be easy to run anew with results that can be combined to reduce the variance
- 2. Sources of errors must be controllable/isolatable
 - ▶ Programming/science errors under your control
 - ▶ Make possible RNG errors approachable
- 3. Reproducibility
 - ▶ Must be able to rerun a calculation with the same numbers
 - ▶ Across different machines (modulo arithmetic issues)
 - ▶ Parallel and distributed computers?

Early Random Number Generators on Digital Computers

- ▶ Middle-Square method: von Neumann
 1. 10 digit numbers: $x_{n+1} = \lfloor \frac{x_n^2}{10^5} \rfloor \pmod{10^{10}}$
 2. Multiplication leads to good mixing
 3. Zeros in lead to short periods and cycle collapse
- ▶ Linear congruential method: D. H. Lehmer
- ▶ $x_{n+1} = ax_n + c \pmod{m}$
- ▶ Good properties with good parameters
- ▶ Has become very popular

What are Random Numbers Used For?





- ▶ There are many types of random numbers
 1. “Real” random numbers: a mathematical idealization
 2. Random numbers based on a “physical source” of randomness
 3. Computational Random numbers
 1. Pseudorandom numbers: deterministic sequence that passes tests of randomness
 2. Cryptographic numbers: totally unpredictable
 3. Quasirandom numbers: very uniform points



Future Work on Random Numbers

1. Support for new architectures
 - ▶ Multicore processors: OpenMP-SPRNG
 - ▶ GPGPU support: LCGs and FLGs
2. Testing Random Numbers
 - ▶ Hardware random numbers
 - ▶ Cryptographic test suites
 - ▶ Support for new RNG suites
3. Applications
 - ▶ Monte Carlo on new architectures
 - ▶ Reproducibility and system integrity
 - ▶ Computational resilience and fault tolerance
4. Commercialization of SPRNG

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Questions?

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