Monte Carlo Methods: Early History and The Basics

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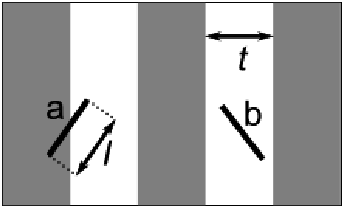
Outline of the Talk

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
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

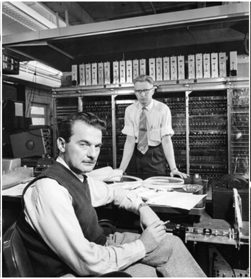
- Los Alamos brought together many interesting factors to give birth to modern Monte Carlo algorithms
    1. The Problems: Simulation of neutron histories (neutronics), hydrodynamics, thermonuclear detonation
    2. The People: Enrico Fermi, Stan Ulam, John von Neumann, Nick Metropolis, Edward Teller, ...
    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

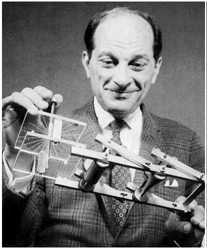
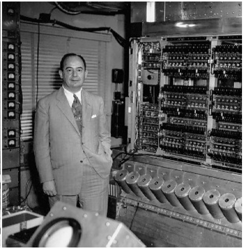
The People

- 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

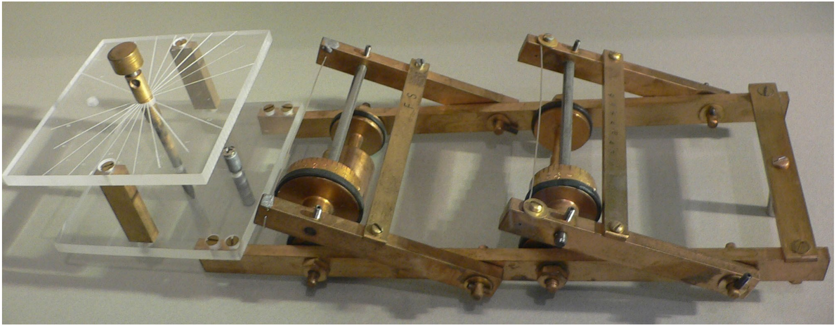


Figure: A Fermiac at the Bradbury Science Museum in Los Alamos

An Analog Monte Carlo Computer: The Fermiac

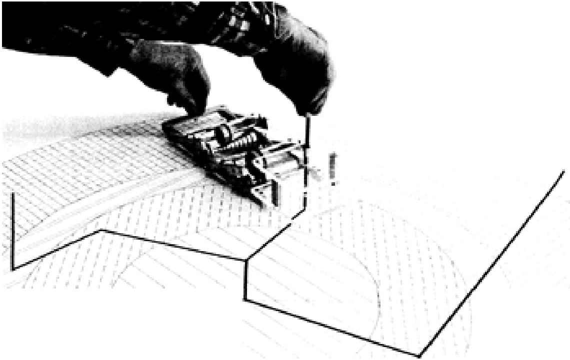


Figure: The Fermiac in Action

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

Figure: The ENIAC at the University of Pennsylvania

An Early Digital Computer: The ENIAC

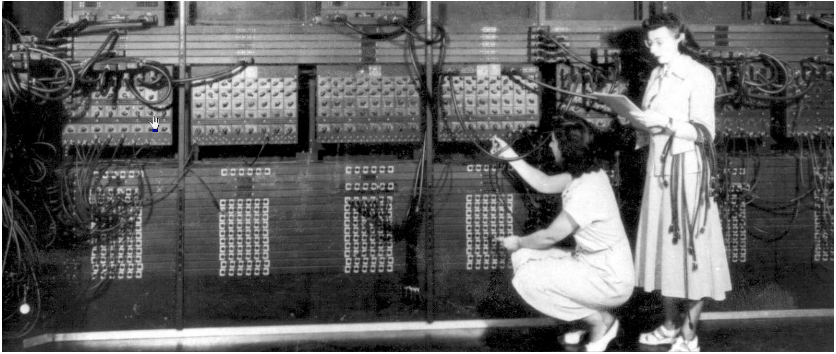


Figure: Programming the ENIAC

An Early Digital Computer: The ENIAC

Figure: Tubes from 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 (NIST), Oak Ridge
  2. 1954, Gainesville, FL: University of Florida Statistical Lab

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:

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

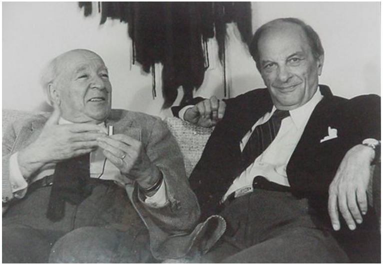
  and in particular we have $x^k = \sum_{i=0}^{k-1} H^i b$, and similarly the Neumann series converges:

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

- 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

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Questions?