

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

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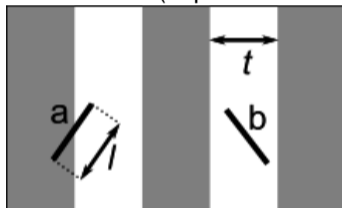
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 4. 1812: Laplace, *Théorie Analytique des Probabilités*

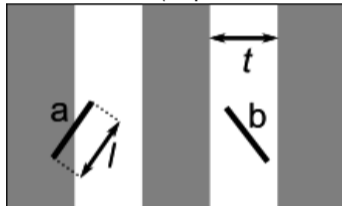
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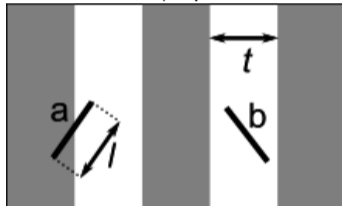
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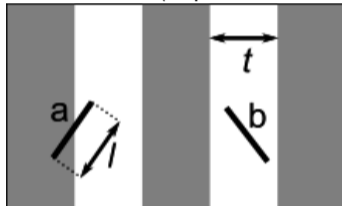
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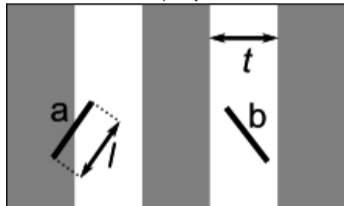
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- ▶ In the 1930's, Fermi used sampling methods to estimate quantities involved in controlled fission

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- ▶ The Name: Ulam's uncle would borrow money from the family by saying that "I just have to go to Monte Carlo"

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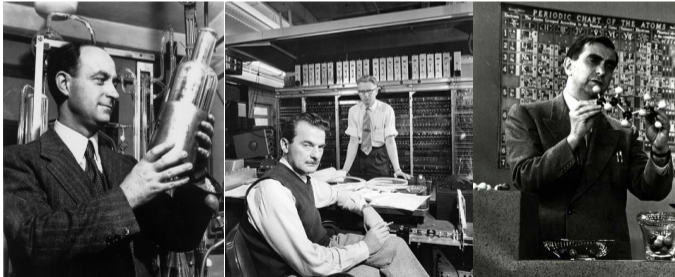
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 2. Geometry is problematic for deterministic methods but not for MC



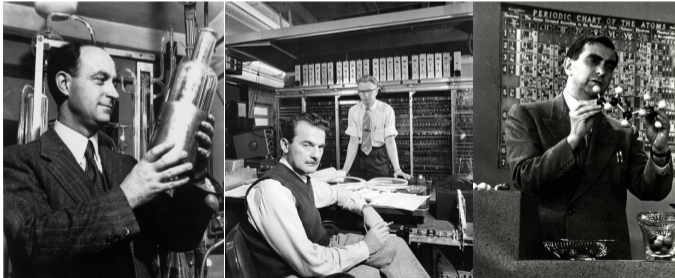
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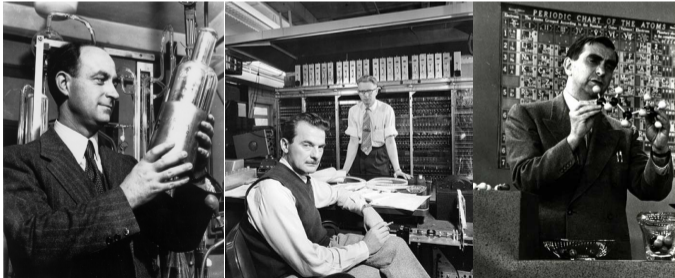
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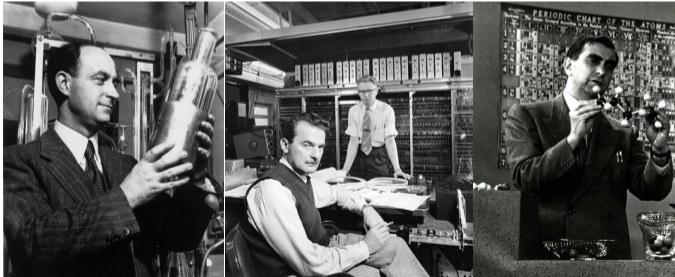
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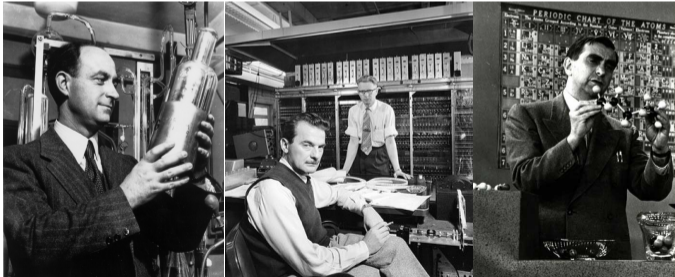
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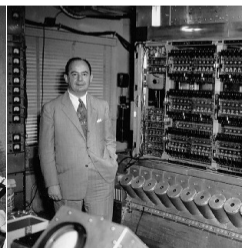
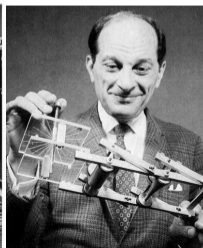
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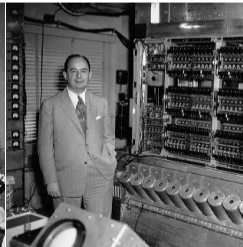
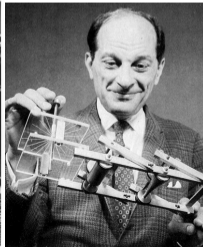
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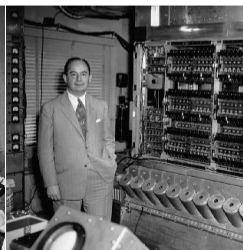
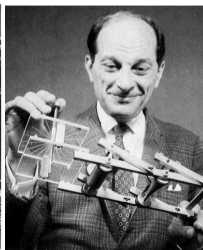
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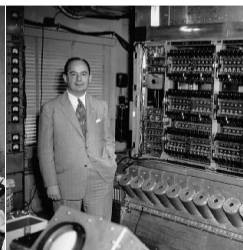
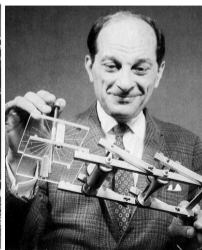
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3. John von Neumann: devised Monte Carlo algorithms and helped develop digital computers



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 4. Continued development and acquisition of digital computers by Metropolis including the MANIAC

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- ▶ Parallelism is achievable with the Fermiac

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

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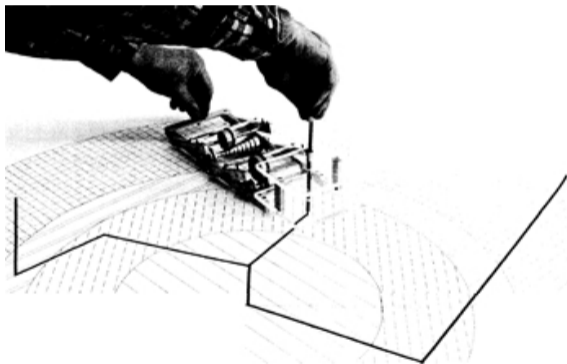


Figure: The Fermiac in Action

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- ▶ Remained in continuous operation at the Army BRL until 1955



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- ▶ Metropolis would go to BRL to work on the “Los Alamos” problem on the ENIAC



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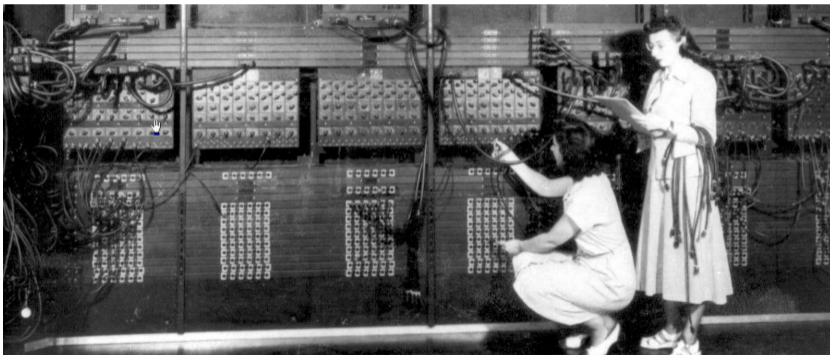


Figure: Programming the ENIAC

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 2. 1954, Gainesville, FL: University of Florida Statistical Lab

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- ▶ 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

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

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

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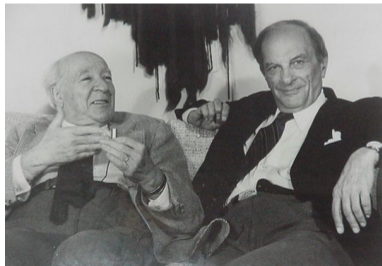
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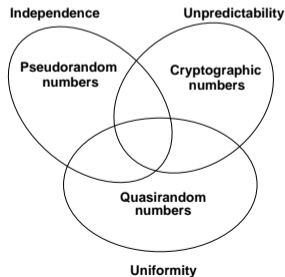
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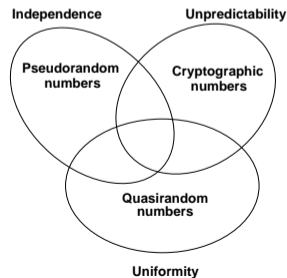
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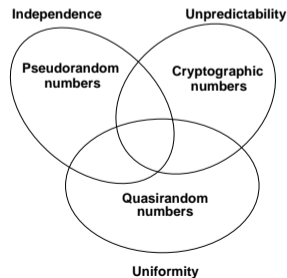
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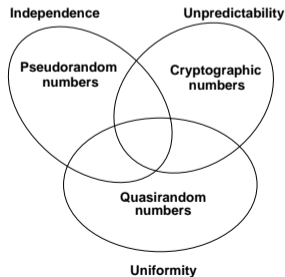
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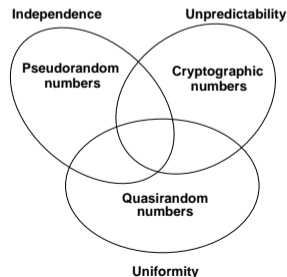
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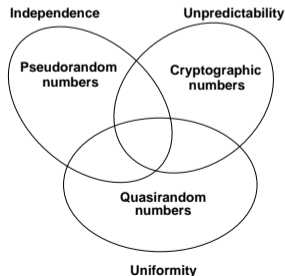
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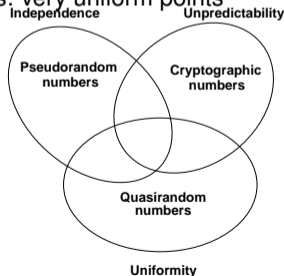
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4. Commercialization of SPRNG



References



[M. Mascagni, T. Anderson, H. Yu and Y. Qiu (2014)]
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References

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-  [M. Mascagni and A. Srinivasan (2000)]
Algorithm 806: SPRNG: A Scalable Library for Pseudorandom Number Generation,
ACM Transactions on Mathematical Software, **26**: 436–461.



Questions?

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