Monte Carlo Simulations I. Introduction

Y. Yin

Monte Carlo simulations

- Randomness and MC
- Key elements in Monte Carlo simulations
- Some practical examples of MC
- Simple MC tutorial

Monte Carlo (MC) simulations

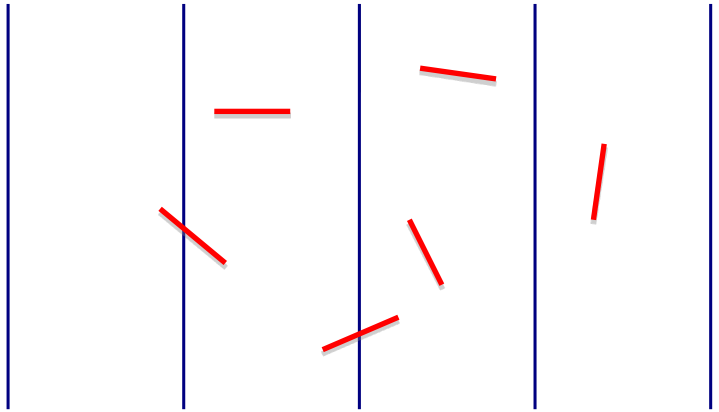
- Refers to a broad class of computational methods that rely on **random statistical sampling**
- Uses random numbers (Monte Carlo is the casino capital of Monaco)
- Initial developed in statistical physics
- Adapted for materials phenomena, in particular grain growth and phase transformations

John von Neumann

Monte-Carlo, Monaco

Buffon's needle problem (1777)

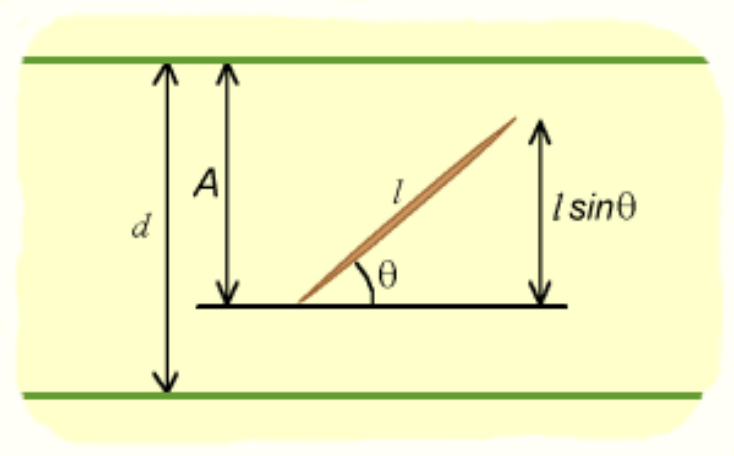
- Used to approximate the number π
- *Problem: find the probability that a needle of length L will land on a line, given a floor with equally spaced parallel lines at distance d apart.*



Drop a need on the surface -> not intersect / intersect with line
The randomness of the problem means that any position of the needle are equally probable.

Mathematical Solution

- The probability of intersection can be mathematically expressed by:
- $P_{intersect} = 2l/\pi d$
- If we randomly drop the need N times and in these drops the needle intersects with the line M times, then the fraction of intersection is
- $P_{intersect} = M/\mathrm{N}$
- Then π can be estimated by $\pi = 2lN/dM$



Statistical Sampling of the Buffon's Problem

Experiments	Year	Needle Length	Sample Size	Intersected Sample	Estimated π
Wolf	1850	0.8	5000	2532	3.1596
Smith	1855	0.6	3204	1218	3.1554
De Morgan	1860	1.0	600	382	3.137
Fox	1884	0.75	1030	489	3.1595
Lazzerini	1901	0.83	3408	1808	3.1415929
Reina	1925	0.5419	2520	859	3.1795

$$\pi = \frac{2lN}{dM}$$

Lessons from Buffon: Important Steps in Monte Carlo Simulation

General	Mathematical
Formulate a probabilistic analogue of the problem	Formulate integral expressions of the governing differential equations that describe the stochastic process
Apply a Monte Carlo algorithm	Integrate the governing expression using a weighted or nonweighted random sampling method
Present and interpret results	Extract state equation values, correlation functions, structural information, or MC kinetics

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Basic Concepts of Monte Carlo Simulations

- The objective of Monte Carlo simulations is to find the probability of a certain event, or the mathematic expectation of a certain random variable, or a related parameter.

- Monte Carlo simulations can be used to solve deterministic problems (e.g. calculate multiple integral, or solve differential equation), as well as nondeterministic problems (i.e. problems with randomness involved) (e.g. nuclear physics, materials physics problems)

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- Due to the extensive employment of stochastic sampling, the development of the Monte Carlo method was closely connected with the progress in computational technology.

A General Algorithm for MC

- 1. We start with a system of N particles and calculate its energy E.

- 2. Select one random particle and give it a random displacement, and calculate the energy of the system after the move, denoted as E'.

- 3. Accept the move if E'-E<0
- or exp(kB/T*(E'-E))<1 if E'-E>0

- 4. If accepted, use the new configuration as the base configuration and return to Step 1.
- If rejected, do nothing and return to Step 1.

- 5. The loop is stopped when a certain criterion is meet. Then we regard the system as "relaxed".

Generating Random Numbers (or Random Number Generation, RNG)

- The stochastic character of this method requires input of huge series of uncorrelated random numbers.

- Ways of generating random numbers: Physical Method

Dice

Radio Noise

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- Ways of generating random numbers: Physical Method

Disadvantages:
1. The generated random sequence is not reproducible.
2. The cost of adding new random number generator is expensive.

Generating Random Numbers (or Random Number Generation, RNG)

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- Ways of generating random numbers: Computational Method

TABLE 1 - RANDOM

11164	36318	75061	37674	26320	75100
21215	91791	76831	58678	87054	31687
10438	44482	66558	37649	08882	90870
36792	26236	33266	66583	60881	97395
73944	04773	12032	51414	82384	38370
49563	12872	14063	93104	78483	72717
64208	48237	41701	73117	33242	42314
51486	72875	38605	29341	80749	80151
99756	26360	64516	17971	48478	09610
71325	55217	13015	72907	00431	45117
65285	97198	12138	53010	94601	15838
17264	57327	38224	29301	31381	38109

Ensure probability of sampling of any number in the random number table is equal

Generating Random Numbers (or Random Number Generation, RNG)

- The stochastic character of this method requires input of huge series of uncorrelated random numbers.

- Ways of generating random numbers: Pseudorandom number generator
- Most computer generated random numbers are obtained using this method
- Such algorithms usually start with a number called a **seed** (chosen arbitrarily).

$$x_{n+1} = (ax_n + c)(\mathrm{mod}\, M)$$

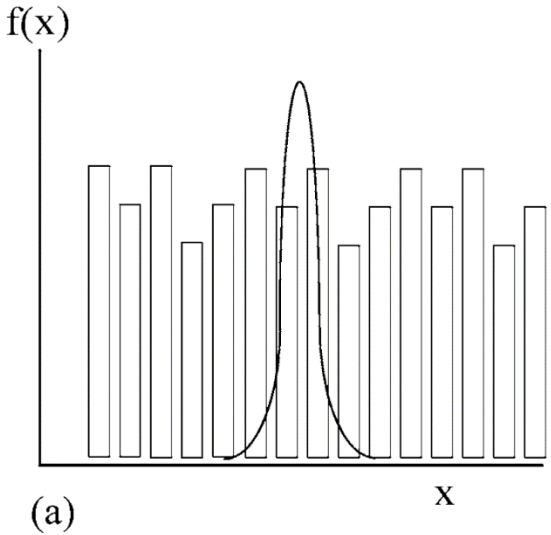
Lehmer method (1951)

$$x_0 = Seed \qquad 0 \le Seed \le 199617$$

$$c = 99991 \qquad a = 24298 \qquad M = 199617$$

Sampling Method: Simple (nonweighted) / Importance (weighted)

- Simple Sampling: use an equal contribution of random numbers



The column indicate the weight frequency
Of chosen x values

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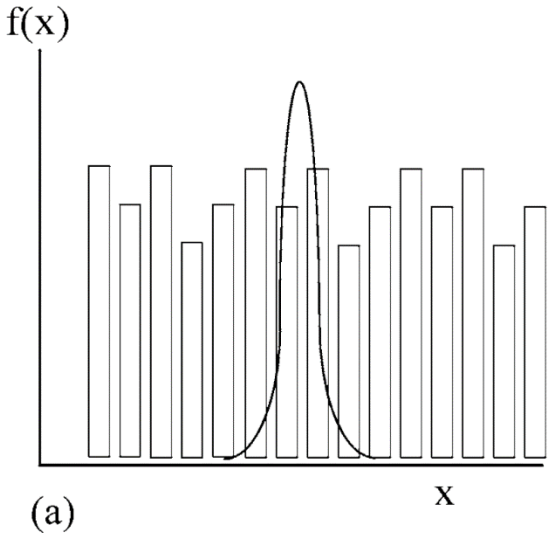

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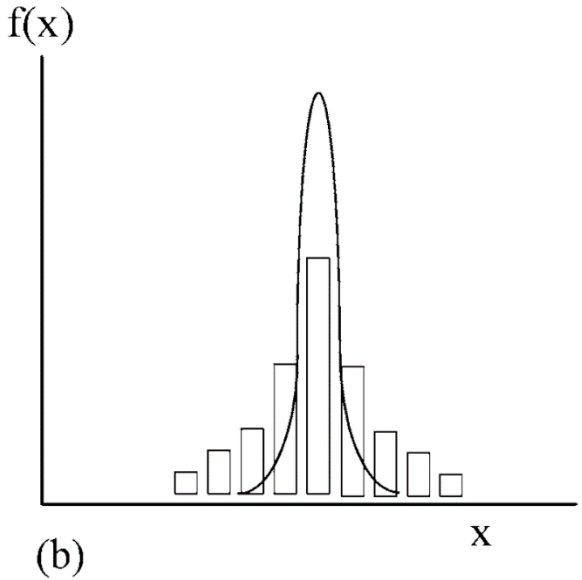
Sampling Method: Simple (nonweighted) / Importance (weighted)

- Importance sampling: Use a distribution accommodated to the problem being investigated.



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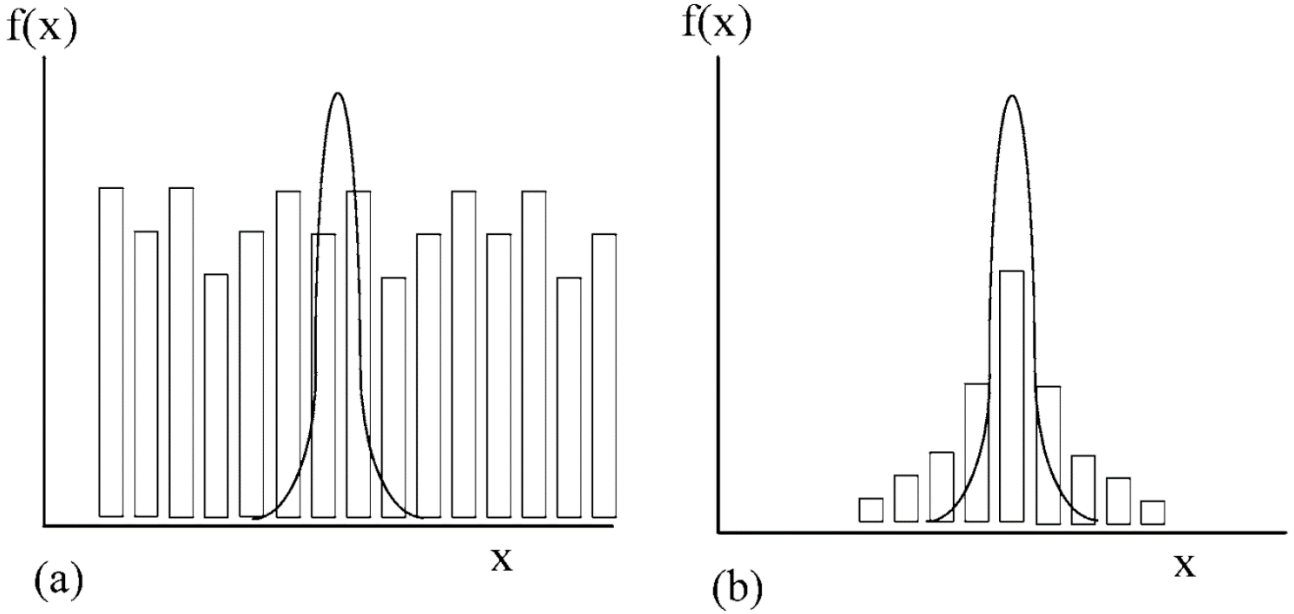
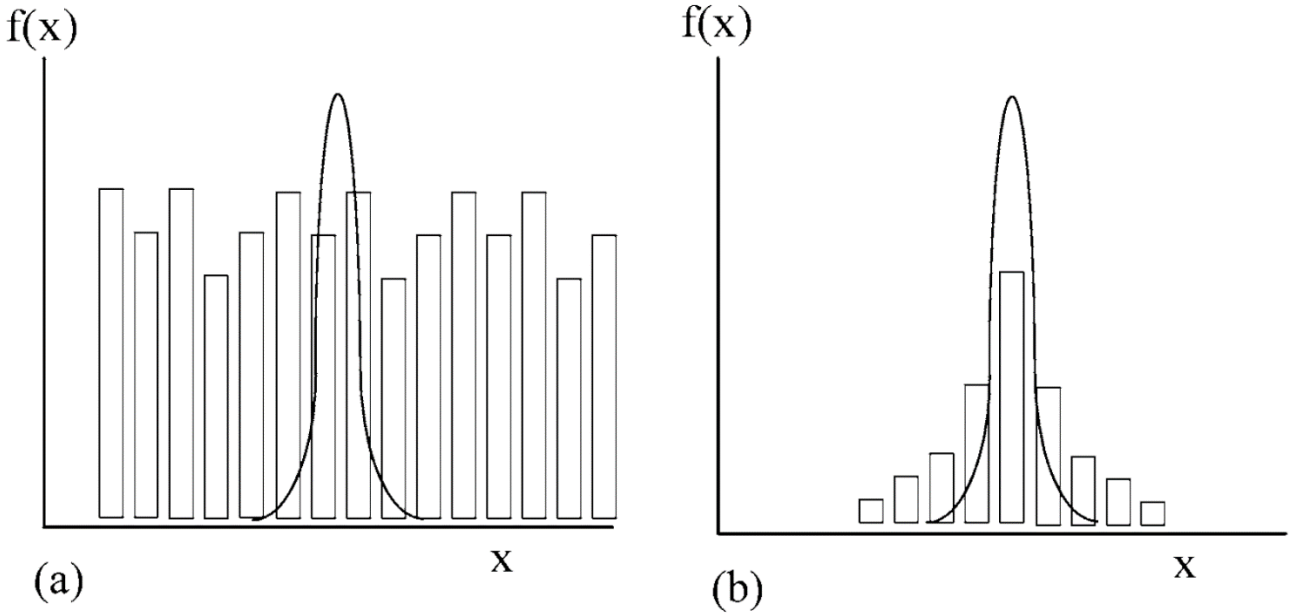
Sampling Method: Simple (nonweighted) / Importance (weighted)

- Simple sampling requires much large number of trais to approximate the true integral than the weighted scheme.



Sampling Method: Simple (nonweighted) / Importance (weighted)

- Therefore Importance sampling is more effective in solving this problem.

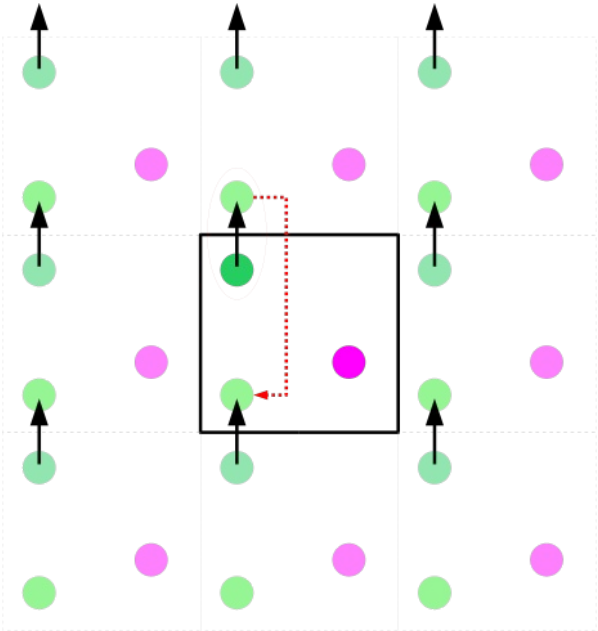


Simple or Importance?

- In practice, the simple sampling techniques is often employed in problems involving integration methods which choose the random numbers from a uniform distribution.
- Most Monte Carlo Simulations in materials science use importance sampling. (e.g membrane growth and graphene edge reconsruction)
- Metropolis Monte Carlo method is the best known algorithm based on importance sampling method (NEXT LECTURE).

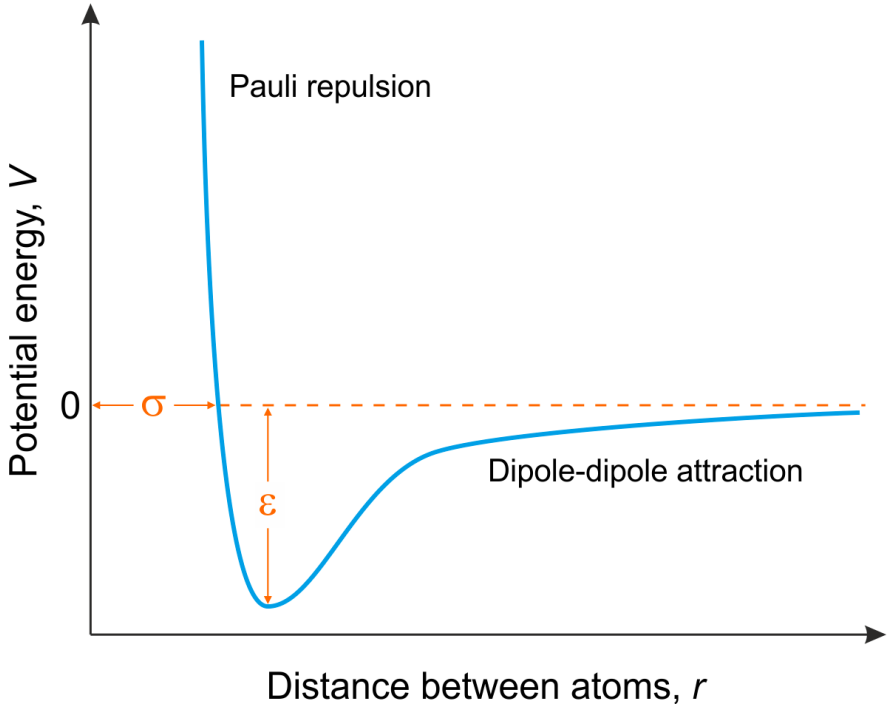
Boundary Conditions

- We usually apply periodic boundary conditions to our simulation box.
- The surface atoms only accounts for a small fraction of total atoms (for a simple cubic crystal of 1000000 atoms, the fraction of surface atoms is only ~6%).
- An effective method for simulating homogeneous bulk systems.



Truncation of Interactions

- Another way to reasonably reduce computational costs.
- Interatomic potentials are usually truncated beyond a critical distance (called cut-off distance), beyond which the interatomic potential is ignored (i.e. regarded as zero).



Summary

- Buffon's Problem – Our 1st Monte Carlo Simulation
- Basic concepts of Monte Carlo Simulations
- Key elements in MC:
- RNG, sampling, boundary conditions, and