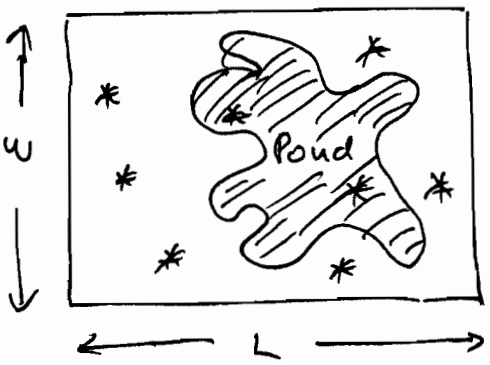
History

Von Neumann, Ulam + Metropolis (1947) → "Studies of diffusion of neutrons in fissionable matter" Coined the term "Monte Carlo"

Metropolis, (Rosenbluth)^2, (Teller)^2 (1953) → First MC simulation for equilibrium stat. mech. properties on hard-disk system.

Monte Carlo Integration



To calculate the area of a pond of arbitrary shape, throw stones at random in W × L area

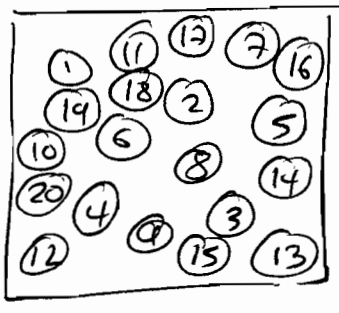
$$\text{Area of Pond} \simeq W \times L \times \frac{(\text{hits in pond})}{(\text{total throws})}$$

Finding an area is an integration problem; Monte Carlo sampling is one way to perform multi-dimensional integrals.

Partition Function

$$Q = \int \cdots \int e^{-\beta U(\vec{r}^N)} d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N$$

Unfortunately, random throws almost always result in overlaps → no contribution to Q



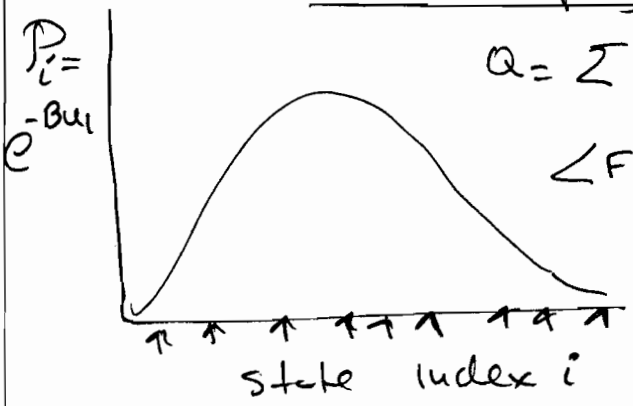
20 particles

Importance Sampling

Also called Metropolis MC. Overcomes sampling problem by generating states with a desired probability distribution, rather than uniformly.

Abandons calculation of Q, instead focuses on calculating averages over ensembles

Uniform sampling

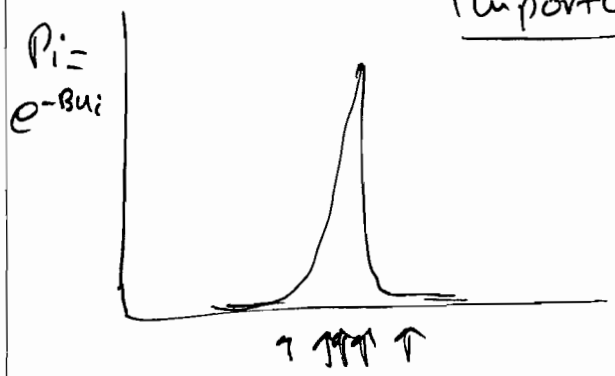


$$Q = \sum P_i$$

$$\langle F \rangle = \frac{\sum (F_i P_i)}{Q}$$

Impractical for most stat. mech. systems

Importance Sampling | with probability proportional to P_i



$$Q = ?$$

$$\langle F \rangle = \frac{\sum F_i}{n}$$

n ↑ number of samples

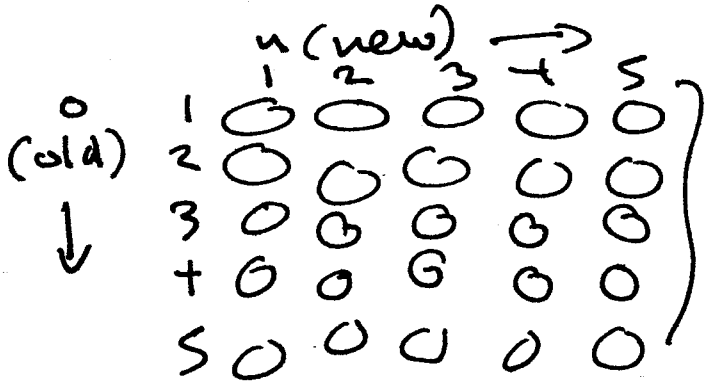
How do we generate states with the correct probability distribution?

→ Impose "detailed balance" condition for transitions between any two states, "o" and "n"

Markov Chain: sequence of states with no memory

E.g. 5-state system $\mathcal{P}_i \propto i$

1, 2, 3, 4, 5



$\underline{\underline{\Pi}}_{(o \to n)}$ elements $\Pi_{(o \to n)}$

TBD

$\alpha(o \to n)$: algorithm, e.g. ⊙ if at i, pick $i+1$

- If at i, pick $\underline{\underline{\text{anything}}}$
- If at i pick $i+2$

etc.

Initial state $\vec{P}_0$

(column vector)

$$\vec{P}_1 = \vec{P}_0^T \cdot \underline{\underline{\Pi}}$$

$$\vec{P}_{n+1} = \vec{P}_n^T \cdot \underline{\underline{\Pi}}$$

$$N(o)\cdot\Pi(o\to n) = N(n)\cdot\Pi(n\to o) \quad (1)$$

$N(o)$: number of states in a very large sample

$\Pi(o\to n)$: probability of transition between states

$$\Pi(o\to n) = \underbrace{\alpha(o\to n)}_{\text{probability of selecting state } n \text{ from state } o,\ \text{contains rules for attempted changes to system}} \times \underbrace{\text{Accept}(o\to n)}_{\text{to be determined by desired statistical ensemble}} \quad (2)$$

$$\Pi(n\to o) = \alpha(n\to o)\times \text{Accept}(n\to o) \quad (3)$$

Need microscopic reversibility $\boxed{\alpha(o\to n) = \alpha(n\to o)}$

Then (1) becomes

$$N(o)\cdot\alpha(o\to n)\cdot\text{Accept}(o\to n) = N(n)\cdot\alpha(n\to o)\cdot\text{Accept}(n\to o)$$

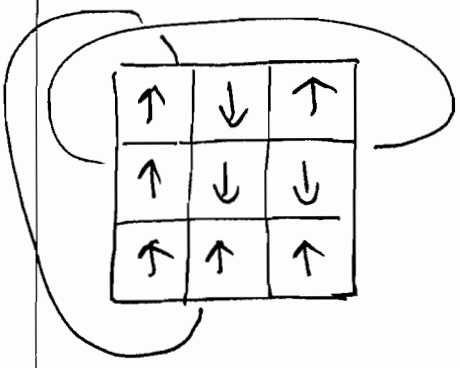
$$\Rightarrow \frac{\text{Accept}(o\to n)}{\text{Accept}(n\to o)} = \frac{N(n)}{N(o)} = \underbrace{\exp(-\beta\Delta u)}_{\text{for canonical (NVT) ensemble}} \quad (4)$$

One (of many) possible ways to satisfy Eq. (4):

Metropolis Rule:

$$\underbrace{\text{Accept}(o\to n)}_{\text{probability of acceptance}} = \begin{cases} 1 & \text{if } \Delta u \le 0 \\ e^{-\beta\Delta u} & \text{if } \Delta u > 0 \end{cases}$$

Example. Ising 2D simulation



periodic boundary conditions to avoid "edge effects"

- start from arbitrary initial configuration
- select a spin at random
- attempt to flip it, calculate Δu
- accept new state with Metropolis rule $P_{acc} = \min\{1, e^{-\Delta u}\}$

Q's: Would it be ok to:

(a) select more than 1 spins to flip?

(b) go over all spins in sequence, rather than picking them randomly?

Typical Monte Carlo Trajectory