Monte-Carlo methods

경상국립대학교 수학과 석사과정 오서영

Background

Monte-Carlo methods

- Goal : sampling of a process in order to determine some statistical properties
- ex) toss a coin 4 times -> probability of 3 tail, 1 head

→ Mathematical solution : $p(3\ head) = \binom{4}{3}\left(\frac{1}{2}\right)^3\left(1-\frac{1}{2}\right)^1 = \frac{1}{4}$

→ **Simulation!**

Python simulation

```python
from random import randint

success = 0

attempts = 10000
for i in range(attempts):
    if randint(0,1)+randint(0,1)+randint(0,1)+randint(0,1) == 3:
        success +=1

print("Number of attempts :", attempts)
print("Number of success :", success)
```

```
Number of attempts : 10000
Number of success : 2464
```

Markov-chain Monte-Carlo

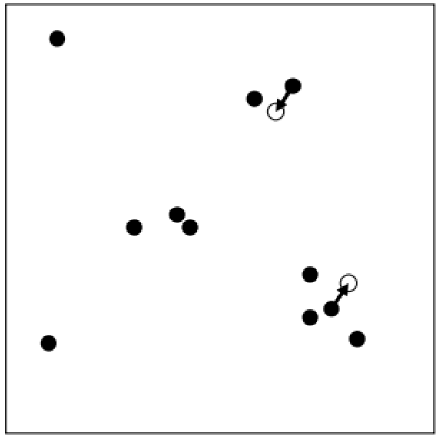
Markov-chain Monte-Carlo (MCMC)

We consider a stochastic process whose goal is to explore the state space of interest

- Let x be a point in this state space
- Assume that x moves across the space by jumping randomly to another point x'

→ This jump takes place with probability $W_{x\to x'}$ → transition function

→ This advanced the system time from t to t+1 Markov chain



We want this process to sample a prescribed probability $\rho(t,x)$

→ How to choose $W_{x\to x'}$

Markov-chain Monte-Carlo

Sampling the diffusion equation

The probability that our random exportation is at x at time t

: $p(t+1,x) = \sum_{x'} p(t,x') W_{x' \to x}$

Let $x \in Z$ 1D discrete space

- W_+: probability to move to the right
- W_- : probability to move to the left
- W_0: probability to stay

→ $p(t,x)$ simplifies to

: $p(t+1,x) = p(t,x-1)W_+ + p(t,x)W_0 + p(t,x+1)W_-$

Markov-chain Monte-Carlo

Diffusion equation

: $\partial_t \rho = D\partial_x{}^2 \rho$

discretize

→ $\rho(t+\Delta t, x) = \rho(t,x) + \frac{\Delta t D}{\Delta x^2}(\rho(t,x-1) - 2\rho(t,x) + \rho(t,x+1))$

↕ comparison

$$p(t+1,x) = p(t,x-1)W_+ + p(t,x)W_0 + p(t,x+1)W_-$$

In order to $p = \rho$

$W_+ = W_- = \frac{\Delta t D}{(\Delta x)^2}$ and $W_0 = 1 - 2\frac{\Delta t D}{(\Delta x)^2}$ = 1- W_+- W_-

thus $\frac{\Delta t D}{(\Delta x)^2} \leq \frac{1}{2}$

Markov-chain Monte-Carlo

Monte-Carlo simulation of Diffusion

- A random walk is a way to sample a density ρ that obeys the diffusion equations
- With a random walk, it is easy to add obstacles, or aggregation processes,

hard to include in the DE

Master Equation

The probability to find the random exploration at x at time t is $p(t, x)$ given by

$$\begin{aligned}
p(t+1,x) &= \sum_{x'} p(t,x')W_{x'\to x} \\
&= \sum_{x'\neq x} p(t,x')W_{x'\to x} + p(t,x)W_{x\to x} \\
&= \sum_{x'\neq x} p(t,x')W_{x'\to x} + p(t,x)(1-\sum_{x'\neq x} W_{x\to x'}) \\
&= p(t,x) + \sum_{x'\neq x} [p(t,x')W_{x'\to x} - p(t,x)W_{x\to x'}]
\end{aligned}$$

Markov-chain Monte-Carlo

Detailed balance

In steady state, the condition $p(x) = \rho(x)$ requires that

$$\sum_{x \neq x'} [\underline{\rho(x')W_{x' \to x} - \rho(x)W_{x \to x'}] = 0}$$

Detailed balance condition

Then we can choose $W_{x \to x'}$ according to the detailed balance condition

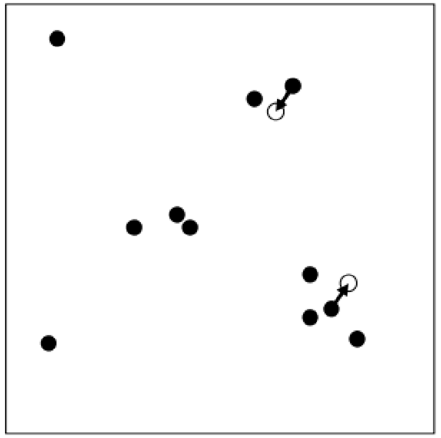
Markov-chain Monte-Carlo

Metropolis Rule

Consider physical system at equilibrium whose probability to be in state x is given by Maxwell-Boltzmann distribution

$$\rho(x) = \Gamma \exp(-\frac{E(x)}{kT})$$

Sample this distribution with a stochastic process by choosing $W_{x \to x'}$ according to the Metropolis rule :



$$W_{x\to x'} = \begin{cases} 1 & E' < E \\ \exp[-(E'-E)/kT] & E' > E \end{cases}$$

$$rand(0,1) < \min(1, \exp\left[-\frac{E'-E}{kT}\right])$$

Markov-chain Monte-Carlo

Metropolis obeys the detailed balance

Let E′>E. Detailed balance is obeyed

$$
(\because) \quad \begin{aligned} \rho(x)W_{x\to x'} &= \Gamma \exp(-E/kT)\exp[-(E'-E)/kT] \\ &= \Gamma \exp(-E'/kT) \\ &= \rho(x') \times 1 \\ &= \rho(x')W_{x'\to x} \end{aligned}
$$

Similarly, if E′≤E

Kinetic / Dynamic Monte-Carlo

Chemical equations

$A \xrightarrow{k_1} B \qquad B \xrightarrow{k_2} A$ Ordinary equation $\longrightarrow$ $\frac{d}{dt}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$

Analytical solution

$$A(t) = \frac{k_2}{k_1 + k_2}(A_0 + B_0) + \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t}$$

$$B(t) = \frac{k_1}{k_1 + k_2}(A_0 + B_0) - \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t}$$

Where A_0 *and* B_0 are the initial concentration of A and B

When $t \to \infty$,

$$A \to A_\infty = \frac{k_2}{k_1 + k_2}(A_0 + B_0) \qquad B \to B_\infty = \frac{k_1}{k_1 + k_2}(A_0 + B_0)$$

Kinetic / Dynamic Monte-Carlo

Monte-Carlo Simulation

1. Time step Δt,

$k_1\Delta t, k_2\Delta t$<1

: probabilities that during Δt, one A particle get transformed into B particle, or conversely

2. Choose randomly a particle among the N=A(t)+B(t)=const of them

(Choose A particle rand(0,1)<A/(A+B), and B particle otherwise.

3. If A particle was chosen, it is transformed into B particle provided

rand(0,1) < $k_1\Delta t$ then A=A-1, B=B+1

If B particle was chosen, it is transformed into A particle provided

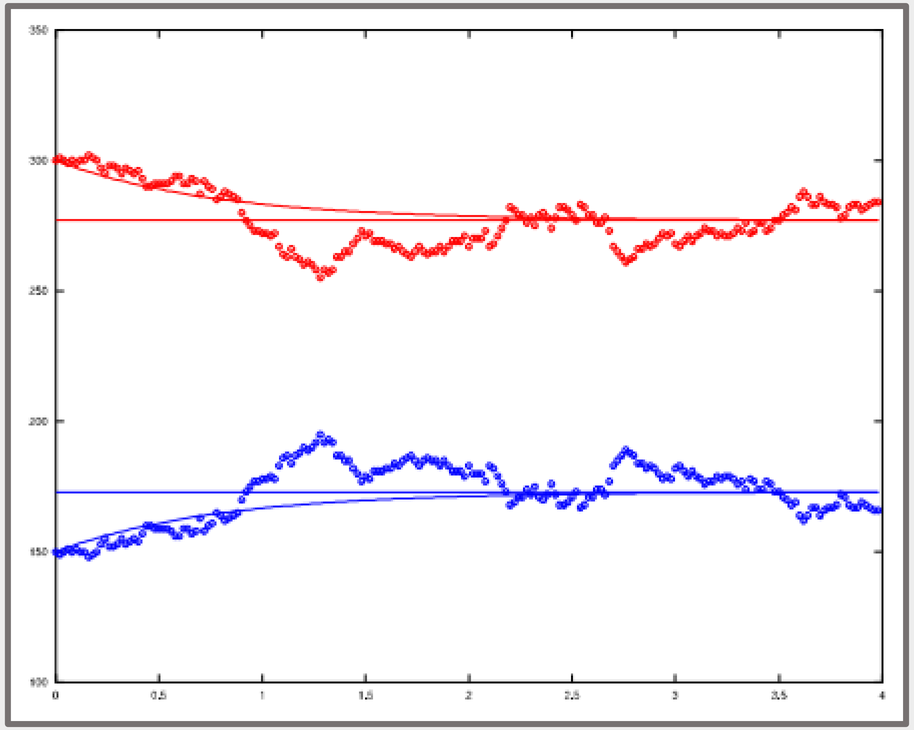
rand(0,1) < $k_2\Delta t$ then A=A+1, B=B-1

4. Repeat **1, 2** for N times and the physical time t is incremented by Δt ($t = t + \Delta t$)

5. Repeat **2~4** until $t = t_{max}$

Kinetic / Dynamic Monte-Carlo

Results



Fluctuation around analytic solution
-> We should average over several runs

References

[1] Simulation and modeling of natural processes, University of Geneva, Coursera

[2] Markov Chain Monte Carlo, https://angeloyeo.github.io/2020/09/17/MCMC.html