Lecture October 23

MC - integration

1-dim

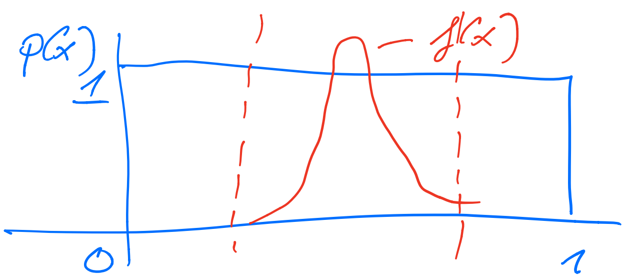
$$\int_a^b f(x)\,dx \simeq \frac{1}{N}\sum_{i\in D} f(x_i)$$

$$x \in [a,b]$$

$b = 1 \quad a = 0$

PDF = uniform PDF

$$p(x)\,dx = \begin{cases} dx & 0 \le x \le 1 \\ 0 & \text{else} \end{cases}$$



$$\boxed{\int_a^b f(x)\,dx} \qquad \int_a^b p(x)\,dx = 1$$

$$\frac{f(x)}{p(x)} \simeq \text{constant} \Rightarrow \sigma_f^2 \simeq 0$$

importance sampling

$$\boxed{\int_a p(x)\,\frac{g(x)}{p(x)}\,dx = \text{constant}}$$

$$\frac{f(x)}{p(x)} = \text{constant for all } x \in [a,b]$$

$$\int_a^b p(x)\,F(x)\,dx$$

$$F(x) = f(x)/p(x)$$

change of variables

$$\int_0^1 p(y)\,dy = \underline{1}$$

$x(y)$ well defined

$$\int_a^b p(x)\,F(x)\,dx = \int_0^1 F(x(y))\,dy$$

$$\underline{I} = \int_{a_1}^{b_1} dx_1 \int_{a_2}^{b_2} dx_2 \cdots \int_{a_d}^{b_d} dx_d$$

$$\times f(x_1, x_2 \ldots x_d)$$

uniform PDF with $\tilde{x}_i \in [0,1]$

could use a mapping

$$x_i = a_i + (b_i - a_i)\,\tilde{x}_i$$

$$dx_i' = (b_i - a_i)\, d\tilde{x}_i$$

$$f(x_1, x_2, \ldots x_d) = f(a_1 + (b_1 - a_1)\tilde{x}_1, a_2 + (b_2 - a_2)\tilde{x}_2, \ldots)$$

we need a factor

$(b_i - a_i)$ for dx_i' $\Rightarrow$

$$\prod_{i=1}^{d} (\underline{b_i - a_i})$$

Example 6-dim function

$$\int_{-\infty}^{\infty} dx_1\, dy_1\, dz_1\, dx_2\, dy_2\, dz_2\; g(x_1, y_1, z_1, \ldots z_2)$$

$$\boldsymbol{x} = (x_1, y_1, z_1) \quad \boldsymbol{y} = (x_2, y_2, z_2)$$

$$g(\boldsymbol{x}, \boldsymbol{y}) = \underline{\exp(-\boldsymbol{x}^2 - \boldsymbol{y}^2)}(\boldsymbol{x} - \boldsymbol{y})^2$$

a brute force approach:
uniform PDF with $x \in [0,1]$
and map to $-\lambda$ to $+\lambda$
instead of $(-\infty, +\infty)$

$$I \simeq \int_{-\lambda}^{\lambda} \underline{dx_1} \ldots \int_{-\lambda}^{\lambda} \underline{dx_6}\; \underbrace{2^6 \cdot \lambda^6}_{\prod_{i=1}^{6}(b_i - a_i)}$$

$$\times e^{-(x^2+y^2)} (x-y)^2$$

$$x^2 = x_1^2 + y_1^2 + z_1^2$$

<u>Brute force MC.</u>

Importance sampling:

$$e^{-(x^2+y^2)} = e^{-(x_1^2+y_1^2+z_1^2+x_2^2+y_2^2+z_2^2)}$$

$$e^{-x_1^2} = \sqrt{\pi} \frac{1}{\sqrt{\pi}} e^{-x_1^2}$$

a normal PDF with $\mu = 0$ and $\sigma^2 = \underline{1}$

$$I = \pi^3 \int \left(\prod_{i=1}^{6} \frac{1}{\sqrt{\pi}} e^{-x_i^2} \right) \underline{(x-y)^2} \, dx_1 \, dx_2 \ldots dx_6$$

generate random number from $e^{-x_i^2}$ with $x_i \in (-\infty, +\infty)$

$$I \simeq \frac{1}{N} \sum_{i=1}^{N} g(x_i, y_i)$$

$$I = 10,974$$

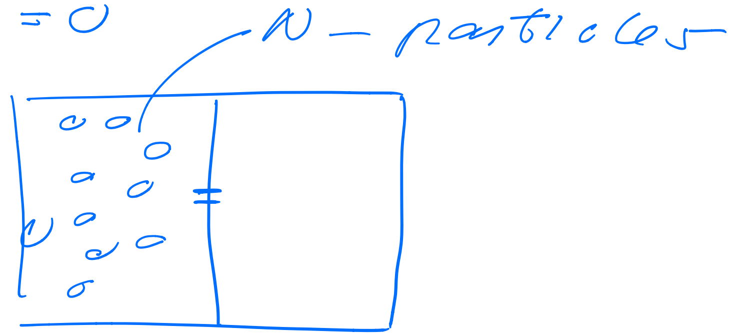
— Markov chains ++ —

chapter 12 of lecture notes

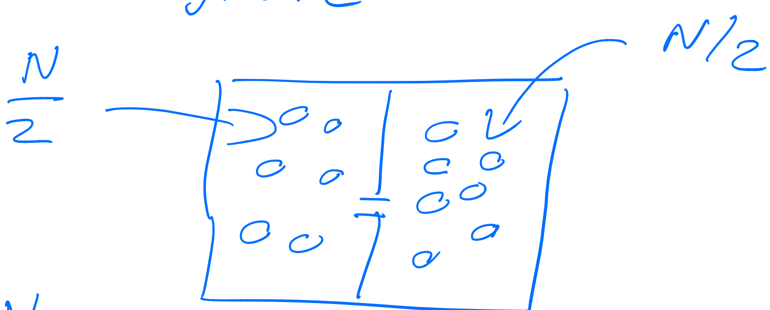
- Basic definition of Markov chain
- Metropolis algo.

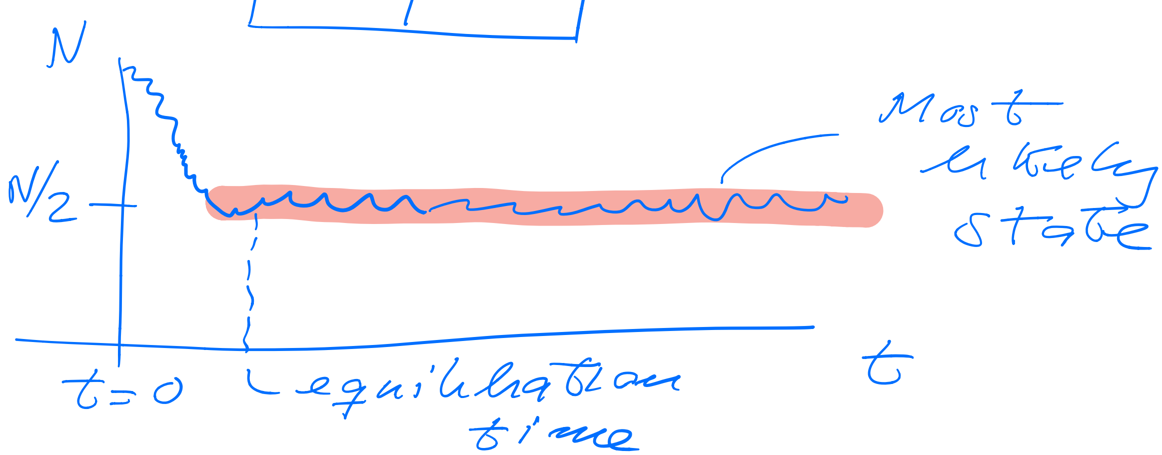
Simple Example: N-particles in a box

$t=0$



t_{final}





Definition of Markov chain

Define a PDF $w(x,t)$ = probability of the system to be in a specific state (x) at time t.

$$w(x,t) \rightarrow w_i(t)$$

i = specific state/configuration

$$\sum_i w_i(t) = 1$$

Transition probability:

$$W(j \rightarrow i) \qquad 0 \leq W_{ij} \leq 1$$

$$\sum_j \underbrace{W(j \rightarrow i)}_{\text{stochastic matrix}} = 1$$

Definition of Markov chain

$$w_i(t+\varepsilon) = \sum_j \underbrace{W(j \rightarrow i)}_{} w_j(t)$$

no time dependence

in matrix vector form

$$w(t+\varepsilon) = W\, w(t)$$

depends only on previous time step. When $t \to \infty$, we reach the most likely state / steady state:

$$\lim_{t \to \infty} \| W(t+\varepsilon) - W(t) \| = 0$$

$\Rightarrow$

$$W w(t=\infty) = w(t=\infty)$$

Eigenvalue problem.

$\underline{\lambda = 1}$

A stochastic matrix W has as its largest eigenvalue $\lambda = \underline{1}$

Problem:

W = unknown or too complicated to evaluate

$w(x,t) = w_i(t)$: we have a model.

P4 : $$w_i(t) = \frac{e^{-E_i/k_B T}}{Z}$$

← normalization constant = partition energy

Metropolis algo comes to our rescue ☺