Monte Carlo Simulations:

Ensemble,

$$\underline{\langle M \rangle} = \sum_i M_i \cdot P_i$$

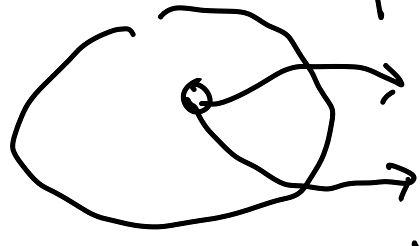
$$= \frac{\int M(p,q)\, e^{-\beta H(p,q)} \cdot dp\, dq}{\int e^{-\beta H(p,q)}\, dp\, dq}$$

$$= \frac{I_A}{I_B}$$

$$I = \int_{a_1}^{b_1} \cdots \int_{a_i}^{b_i} \underbrace{f(x_1, x_2, \cdots)}\ \underbrace{dx_1\, dx_2 \cdots}$$

$$\underbrace{a_1 \cdots a_i}_{V}$$

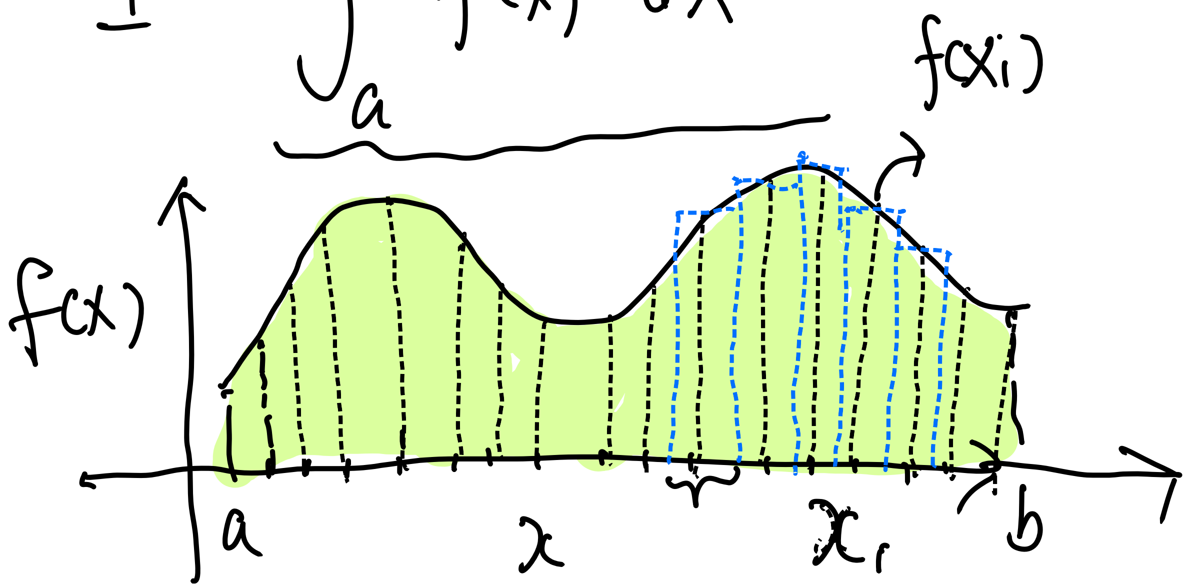
phase space



$dx_1 dx_2 dx_3 \cdots$

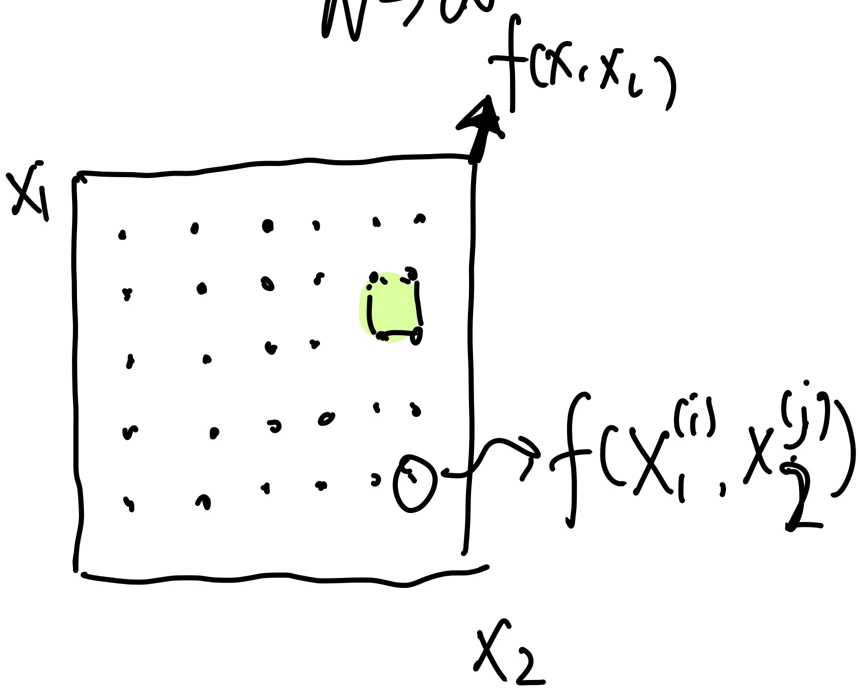
$\underline{f(x_1, x_2, x_3 \cdots)}$

$$I = \int_a^b f(x)\, dx$$



$$\hat{I} = \sum_{i=1}^{N} f(x_i) \cdot \Delta \approx I$$

$$I = \lim_{N \to \infty} \hat{I}$$



$$\hat{I} = \sum_{i=1}^{n} \sum_{j=1}^{n} f(x_1^{(i)}, x_2^{(j)}) \, \Delta_{12}$$

$$\longrightarrow I$$

Simpson's

Quadrature.

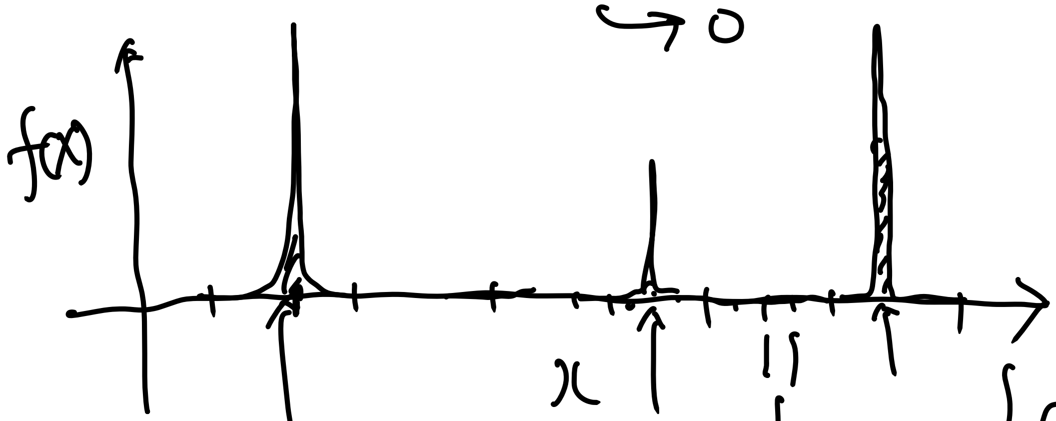
Curse of dimentionality

$N = 10$, $D = 10 \times 6 = 60$

every dim → divide 5 points.

$$\underline{\underline{5^{60}}}$$

$$f(x) \sim \underbrace{e^{-\beta \underbrace{E(x)}}}_{\to 0}$$



$$\hat{I} \neq I$$

$$= \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

$\Delta \sim \delta$ $\quad \boxed{\left(\frac{|b-a|}{\delta}\right)^D}$

$f(x_i) \to 0$

Monte Carlo Simulations:

Inferential Statistics:

Descriptive Stat:

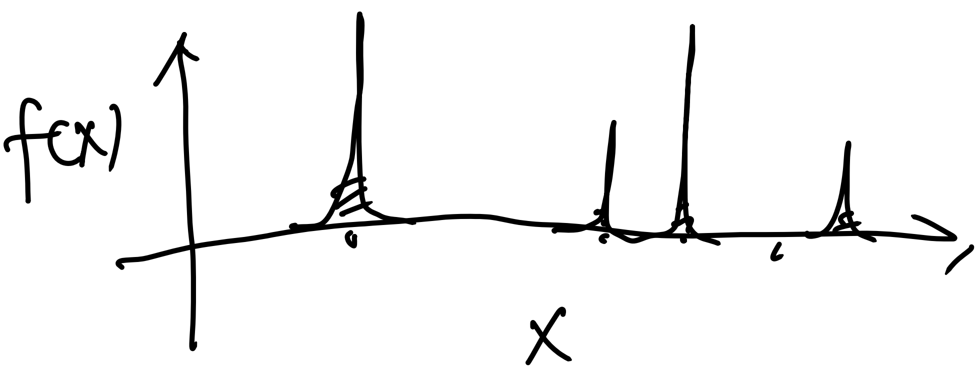
predicition from statistics of data:

① population: all possible states and distribution p_i

② sample: subset of population

③ Random sample can reflect mean properties of the entire population.

④ Law of large Number (Bernoulli's theorem)



$$I = \int_a^b f(x)\,dx = (b-a)\frac{\int_a^b f(x)\,dx}{b-a}$$

$$= b-a\,\frac{\int_a^b f(x)\,dx}{\int_a^b dx} = (b-a)\langle f(x)\rangle$$

x → random variable

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

estimator

$$\hat{I} = (b-a)\frac{1}{L}\sum_{i=1}^{L} f(x_i) \approx I$$

sample

$$\lim_{L\to\infty} \hat{I} = I$$

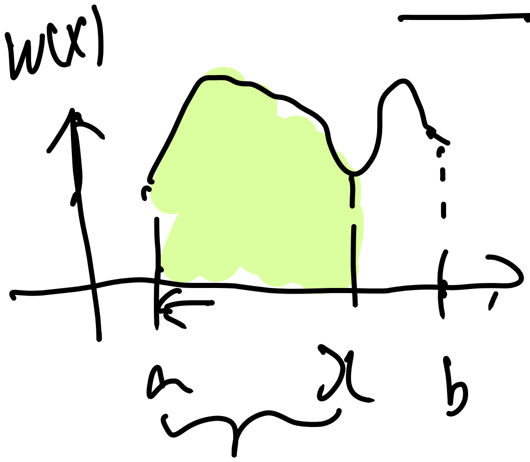
$$I = \int_a^b f(x)\,dx$$

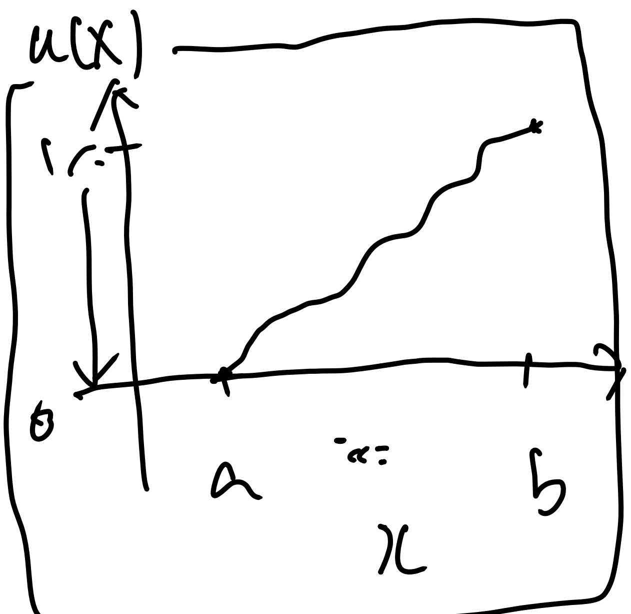
$w(x) \geq 0$

$\int_a^b w(x)\,dx = 1$

$$= \frac{\int_a^b \frac{f(x)}{w(x)}\, w(x)\,dx}{\int_a^b w(x)\,dx} = \left\langle \frac{f(x)}{w(x)} \right\rangle_w$$

define: $u(x) = \int_a^x w(x')\,dx'$ → CDF: cumulative distribution function





$$\frac{du(x)}{dx} = w(x)$$

$$du(x) = w(x)\,dx$$

$$I = \int_a^b \frac{f(x)}{w(x)} \underbrace{w(x)\,dx}_{du} \qquad x \mapsto u$$

$x = u^{-1}(x)$

$$= \int_0^1 \frac{f(x(u))}{w(x(u))} du$$

$$\hat{I} = (1-0) \cdot \frac{1}{L} \sum_{i=1}^{L} \frac{f(x(u_i))}{w(x(u_i))}$$

$u_i \in [0, 1]$

- $\underline{L}$ → fixed

$\hat{I} \longrightarrow I$

Monte Carlo : L , $\hat{I}^{(1)}$ ✓

$\neq$

Monte Carlo : L , $\hat{I}^{(2)}$ ✓

$\vdots$

Monte Carlo : L, $\hat{I}^{(m)}$ ✓

$$\delta^2 = \left\langle \left(\hat{I}^{(i)} - \underset{\sim}{I} \right)^2 \right\rangle_m \qquad m \to \infty$$

$$I$$

$$\delta^2, \quad L, \quad w$$

$$\delta^2 = \left\langle \frac{1}{L} \sum_{i=1}^{L} \left(\boxed{\frac{f(x(u_i^{(k)}))}{w(x(u_i^{(k)}))}} - I \right) \times \frac{1}{L} \sum_{j=1}^{L} \left(\frac{f(x(u_j^{(k)}))}{w(x(u_j^{(k)}))} - I \right) \right\rangle_m$$

$$= \left\langle \frac{1}{L^2} \sum_{i=1}^{L} \sum_{j=1}^{L} \left(\frac{f(x(u_i^{(k)}))}{w(x(u_i^{(k)}))} \cdot \frac{f(x(u_j^{(k)}))}{w(x(u_j^{(k)}))} \to \text{I} \right. - \right.$$

$$\left. \underbrace{I \left(\frac{f(x(u_i^{(k)}))}{w(x(u_i^{(k)}))} + \frac{f(x(u_j^{(k)}))}{w(x(u_j^{(k)}))} \right)}_{\text{II}} + I^2 \right\rangle_m =$$

① $$\left\langle \frac{1}{L^2}\sum_{i\neq j} \frac{f_i^{(k)}}{w_i^{(k)}}\cdot\frac{f_j^{(k)}}{w_j^{(k)}} \right\rangle_m \qquad f_i^{(k)} = f(x(u_i^{(k)}))$$

$$+ \left\langle \frac{1}{L^2}\sum_i \frac{f_i^{(k)2}}{w_i^{(k)2}} \right\rangle_m \qquad k=1,\ldots,m$$

$$= \frac{1}{L^2}\sum_{i\neq j}\left\langle \left\langle\frac{f_i^{(k)}}{w_i^{(k)}}\right\rangle_m \left\langle\frac{f_j^{(k)}}{w_j^{(k)}}\right\rangle \right\rangle_m \hookrightarrow \frac{1}{L^2}\sum_{i\neq j} I^2$$

$$+ \frac{1}{L^2}\sum_{i=1}^{L}\left\langle \frac{f_i^{(k)^2}}{w_i^{(k)2}} \right\rangle_m$$

$$= \frac{1}{L^2}\sum_{i\neq j}\underline{I^2} + \frac{1}{L^2}\sum_{i=1}^{L}\underline{\left\langle\frac{f^2}{w^2}\right\rangle_m}$$

$$= \frac{I^2}{L^2}\cdot L(L-1) + \frac{\left\langle\frac{f^2}{w^2}\right\rangle_m}{L^2}\times L$$

$$= \frac{L-1}{L} I^2 + \frac{1}{L} \left\langle \left(\frac{f}{w}\right)^2 \right\rangle_m$$

$$\text{II} = -\frac{2I^2}{L^2} \cdot L^2 + I^2 = -I^2$$

$$\underline{\underline{\sigma^2}} = \frac{1}{L} \left\langle \left(\frac{f}{w}\right)^2 \right\rangle_m + \frac{L-1}{L} I^2 - I^2$$

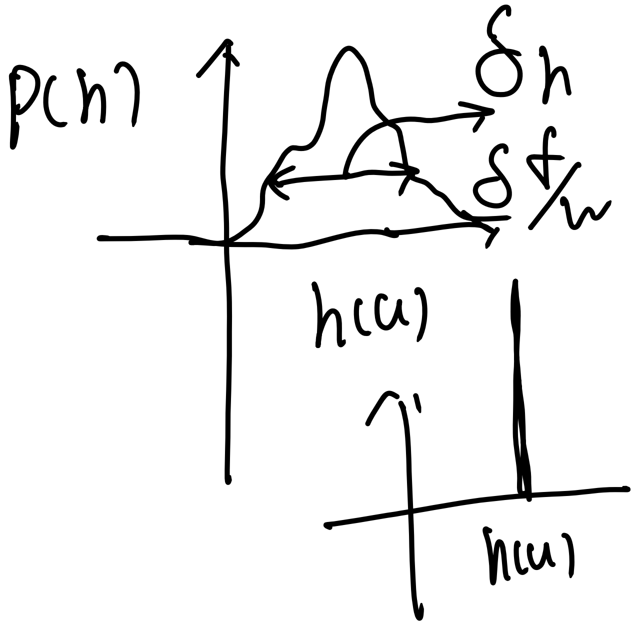
$$= \frac{1}{L} \left(\left\langle \left(\frac{f}{w}\right)^2 \right\rangle_m - \left\langle \frac{f}{w} \right\rangle^2 \right)$$

$$= \frac{1}{L} \underline{\sigma^2_{f/w}}$$

$$\underline{h^{(u)}} = \frac{f(x(u))}{w(x(u))}$$

L $\qquad$ $\underset{\sim}{\sigma^2_{f/w}}$

$\sigma \propto L^{1/2}$



$$\frac{f(x(u))}{w(x(u))} = h(u) = \text{const}$$

$$\hookrightarrow w(x) = \text{const} \cdot \underbrace{f(x)}$$

$$= \text{const} \cdot \underbrace{e^{-\beta H(x)}}$$

MC : L samples. $\vec{q}^{(N)}$, $\vec{q}_i^{(N)}$

n_i

$$\underbrace{n_i} \propto L \cdot \underbrace{p(\vec{q}_i^{(N)})}$$

$$= L \cdot \frac{e^{-\beta U(\vec{q}_i^{(N)})}}{Z}$$

$$\langle M \rangle = \frac{1}{L} \sum_{i=1}^{M} n_i \cdot M(\vec{q}_i^{(N)})$$

two states

i, j

$$\frac{n_i}{n_j} = \frac{\alpha \cdot p(\vec{q}_i)}{\alpha \cdot p(\vec{q}_j)} = \frac{e^{-\beta u(\vec{q}_i)}/Z}{e^{-\beta u(\vec{q}_j)}/Z}$$

$$= e^{-\beta(u(\vec{q}_i) - u(\vec{q}_j))}$$

Transition Probality

$\pi(\vec{q}_i \rightarrow \vec{q}_j)$

Imagine. M MC sampling

for every MC sim

k, sample , $\rightarrow \vec{q}_i, \vec{q}_j$

$\vec{o}, \vec{n}$

$$\hat{p}(\vec{o}) = \frac{m(\vec{o})}{M} \approx p(\vec{o}) = \frac{e^{-\beta u(\vec{o})}}{Z}$$

how about $k+1$

k: $\qquad\qquad\qquad\qquad$ $k+1$:

$$\begin{array}{ccc} \vec{o} & & \vec{n} \\ \vec{o} & & \vec{o} \\ \vec{n} & \longrightarrow & \vec{o} \\ \vec{n} & & \vec{n'} \end{array}$$

$$m^{(k)}(\vec{o}) \longrightarrow m^{(k+1)}(\vec{o})$$

$$\sum_{\{\vec{n}\}} m^{(k)}(\vec{o}) \cdot \pi(\vec{o} \to \vec{n})$$

$$= \sum_{\{\vec{n}\}} m^{(k)}(\vec{n})\, \pi(\vec{n} \to \vec{o})$$ ✓ ✓

✓ $\Uparrow$ $\downarrow$?

$$\frac{m^{(k)}(\vec{o})}{M}\,\underline{\pi(\vec{o}\to\vec{n})}$$

$$= \frac{m^{(k)}(\vec{n})}{M}\,\underline{\pi(\vec{n}\to\vec{o})}$$

detailed balance conditions.

$$p(\vec{o})\,\pi(\vec{o}\to\vec{n}) = p(\vec{n})\,\pi(\vec{n}\to\vec{o})$$

$$\frac{\pi(\vec{o}\to\vec{n})}{\pi(\vec{n}\to\vec{o})} = \frac{p(\vec{n})}{p(\vec{o})} = e^{-\beta(U(\vec{n})-U(\vec{o}))}$$

$$\pi(\vec{o}\to\vec{n}) = \alpha(\vec{o}\to\vec{n})\,\mathrm{acc}(\vec{o}\to\vec{n})$$

$$\frac{\mathrm{acc}(\vec{o}\to\vec{n})}{\mathrm{acc}(\vec{n}\to\vec{o})} = e^{-\beta(U(\vec{n})-U(\vec{o}))}$$

$$\Downarrow$$

$$\mathrm{acc}(\vec{o}\to\vec{n}) = \min\left(1,\ e^{-\beta(U(\vec{n})-U(\vec{o}))}\right)$$

$$\frac{acc(o \to n)}{acc(n \to o)} = \frac{\min(\quad)}{\min(\quad)}$$

MC algorithm:

① Initize randomly select $\vec{O}_0$ $\quad \vec{O}_0 \to \vec{O}$

Repeat {

given $\vec{o}$, generate $\vec{n}$ at random.

generate random displacement $\vec{\Delta}$,

$\vec{n} := \vec{o} + \vec{\Delta}$

calculate $u(\vec{n})$, $f = e^{-\beta(u(\vec{n}) - u(\vec{o}))}$

if $f \geq 1$ accept

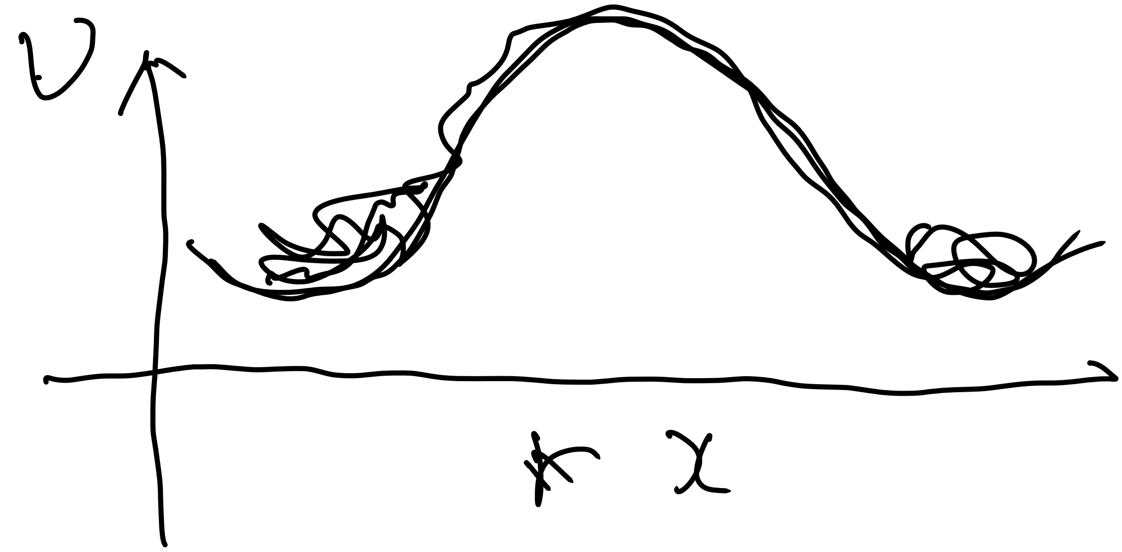
or generate a random number $r \in [0, 1]$

if $r < f$: accept

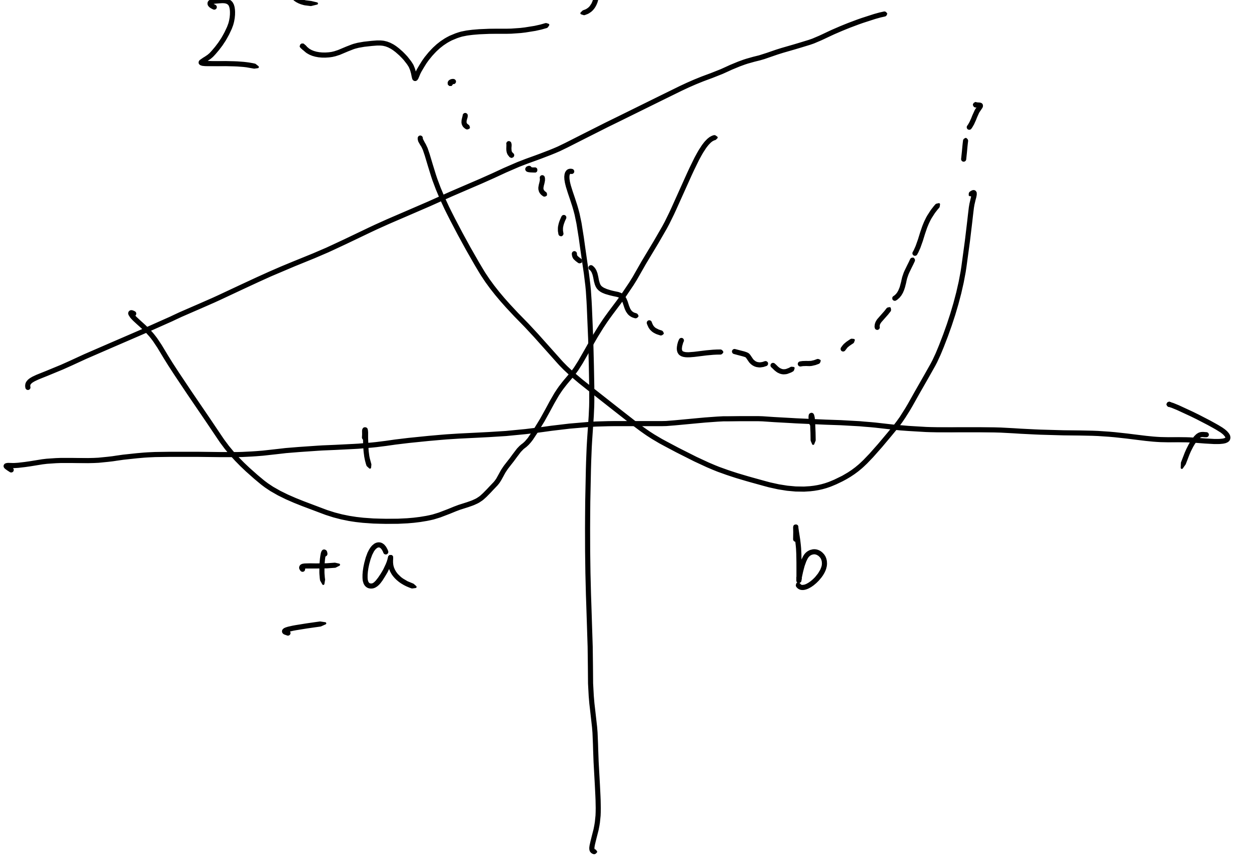
record the current state

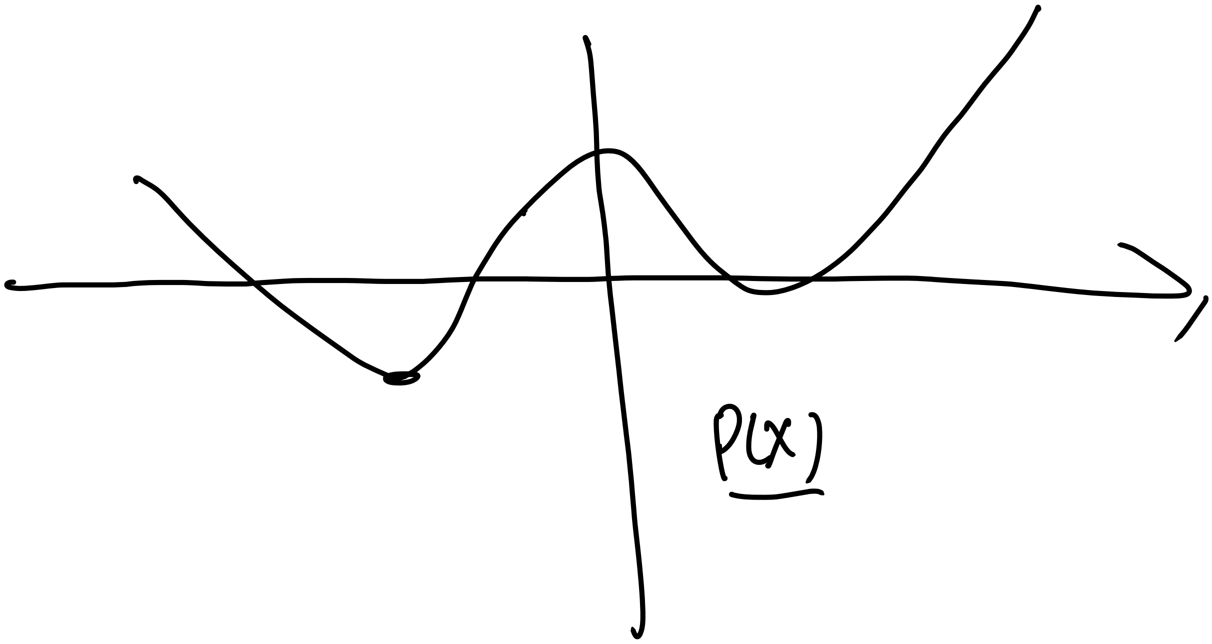
}

1D random walker in a 1D potential energy surface.



$$U = \frac{1}{2}\underbrace{(x+a)^2}\cdot(x-b)^2 + c\cdot X$$





$$\vec{n} = \vec{o} + \vec{\Delta} \in [-a, b]$$

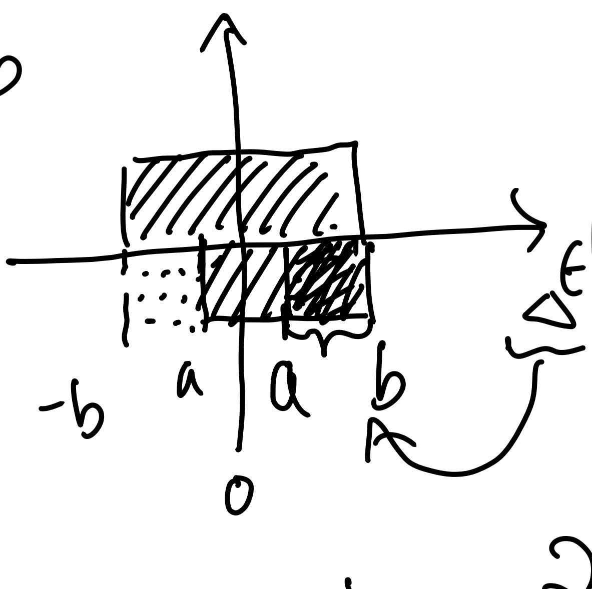
$[-a, a)$

$b = a$

$b \neq a$

$$\partial(\vec{o} \to \vec{n})$$
$$= \partial(\vec{n} \to \vec{o})$$

$a = 0.3b$



$\Delta \in [a, b]$

$$p = \frac{b-a}{b+a}$$

$$\partial(\vec{o} \to \vec{o} + \Delta \in [a, b])$$

$a = 0.3b$

$$\partial(\vec{n} \to \vec{0})$$

$$\Downarrow$$

$$\partial(\vec{0} + \Delta \in [a,b] \to \vec{0})$$

$$\Updownarrow$$

$$\partial(\vec{0} \to \underbrace{\vec{0} - \underline{\Delta} \in [a,b]}_{+\Delta' \in [-b,-a]})$$

$$= 0$$

|a|

$$\vec{0} \longrightarrow \underline{\vec{0}} + \vec{\Delta}$$

$$U(\vec{0})$$

$$U(\vec{0} + \vec{\Delta}) \sim U(\vec{0})$$

$$= U'(\vec{0}) \cdot \vec{\Delta}$$

$\vec{\Delta} \nearrow$ $\quad \Delta U \nearrow$ $\quad$ all $\searrow$

$\vec{\Delta} \downarrow$ slower exploration

$\left| \vec{\Delta}^2 \right|$