Numerical integration : Monte Carlo method

Mathematical problem

$$I = \int d^D x \; f(\vec{x}) \qquad \vec{x} = (x_1, \dots, x_D)$$

$$D \gg 1$$

$$I = \sum_c f_c$$

ex. (1) equilibrium physics of a system of $\underbrace{N \text{ particles in } 3d}_{\{x_i,\, p_i\}}$

$\{x_i, p_i\}$ $\quad i = 1, \dots, 3N$

$$\beta = \frac{1}{k_B T} \qquad D = 6N$$

$$\langle O(\{x_i, p_i\}) \rangle = \frac{\overbrace{\int \left(\prod_i dx_i\right) \left(\prod_i dp_i\right)}^{6N - \text{d.o.f.}} O(\{x_i, p_i\})\, e^{-\beta H(\{x_i, p_i\})}}{\int (\;)(\;)\, e^{-\beta H}}$$

Z

(2) Ising model

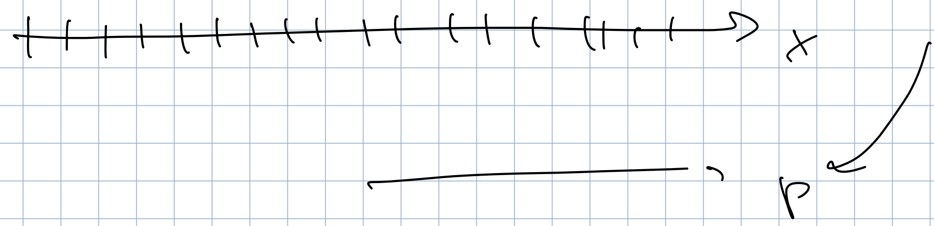
$$\uparrow \; \downarrow \; \uparrow \; \uparrow \; \downarrow$$

$\sigma_i = \pm 1$

2^N

$$\langle o(\{\sigma_i\}) \rangle = \frac{\sum_{\vec{\sigma} = (\sigma_1 \sigma_2 \cdots \sigma_N)} e^{-\beta H(\vec{\sigma})}\, o(\vec{\sigma})}{\sum_{\vec{\sigma}} e^{-\beta H(\vec{\sigma})}}$$

δx d L cells



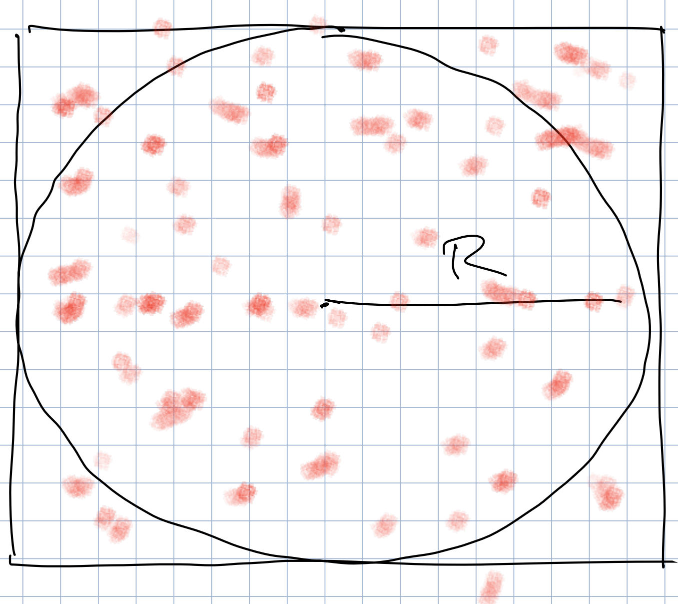
# of cells in phase space : L^{6N}

Numerical integration using stochastic method

draw a "random" sample

A bit history   Buffon's needle problem

Estimating π



$$f = \frac{M_d}{M} \underset{M \to \infty}{\simeq} \frac{\pi R^2}{(2R)^2} = \frac{\pi}{4} = p$$

$\bar{f} = p$ $n = Mf$: number of events of one type

$f = \frac{n}{M}$

$$P(n,M) = \binom{M}{n} p^n (1-p)^{M-n}$$

$$\langle n \rangle = pM$$

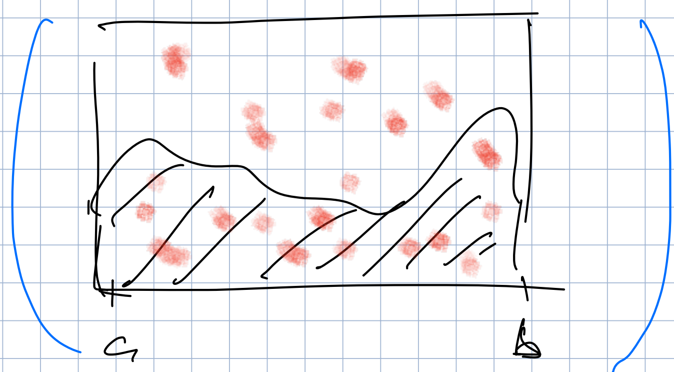
$$\sigma_f^2 = \frac{\sigma_n^2}{M^2} = \frac{\langle n^2 \rangle - \langle n \rangle^2}{M^2} = \frac{M\,p(1-p)}{M^2} = \frac{p(1-p)}{M}$$

$$f_M = \frac{n}{M} \simeq p \pm \sqrt{\frac{\sigma_n^2}{M^2}} = p \pm \sqrt{\frac{p(1-p)}{M}}$$

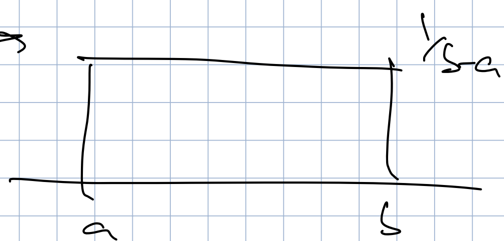
$$= p + \mathcal{O}\left(\frac{1}{\sqrt{M}}\right)$$

Random sampling of integrals

$$I = \frac{1}{b-a}\int_a^b dx\, f(x)$$



$$= \int_a^b dx\, \underbrace{p(x)}_{\frac{1}{b-a}}\, f(x)$$



Idea: draw points in $[a,b]$ with probability $p(x)$

$$x_1, x_2, \dots, x_M \qquad f_i = f(x_i)$$

$$f_1, f_2, \dots, f_M$$

$$I_M = \frac{1}{M}\sum_{i=1}^{M} f_i \underset{M\to\infty}{\simeq} I = \langle f \rangle_p$$

I_M can be regarded as a sum of random variables

$\to$ also a random variable

$$\overline{I_M} = \frac{1}{M} \Sigma_i \overline{f_i} \qquad \to \overline{f_i} = I = \langle f \rangle_p$$

$$= I \qquad \sigma_f^2 = \langle f^2 \rangle_p - \langle f \rangle_p^2$$

$$\boxed{|I_M - \overline{I_M}| \simeq \sigma_{I_M} = \frac{\sigma_f}{\sqrt{M}}}$$

it applies to any dimensions for our integral

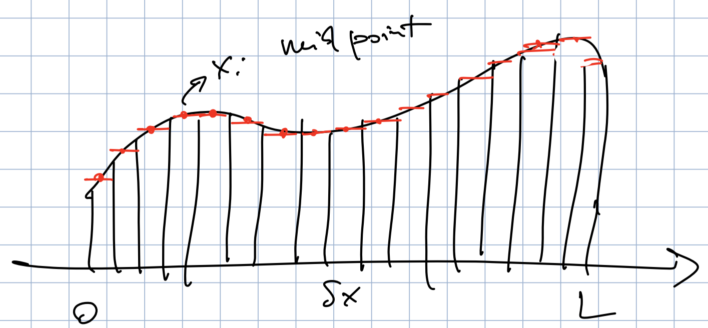
Central limit theorem $\leftarrow$

$$\sigma^2_{\Sigma_i f_i} = M \sigma_f^2$$

$$\sigma_{I_M}^2 = \frac{\sigma_f^2}{M}$$

$\uparrow$

"Deterministic" integration



$$M = \frac{L}{\delta x}$$

$$\delta x = \frac{L}{M}$$

$$I_M - I = \Sigma_i \left(f(x_i)\,\delta x - \int_{x_i - \frac{\delta x}{2}}^{x_i + \frac{\delta x}{2}} dx\, f(x) \right)$$

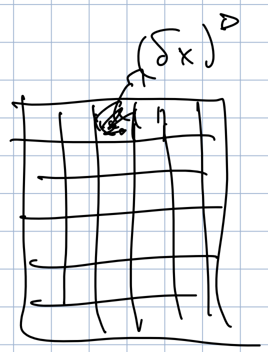
$\uparrow$

$$f(x_i) + \cancel{f'(x_i)(x - x_i)}$$
$$+ \frac{1}{2} f''(x_i) (x - x_i)^2 + \dots$$

$$= M\, O(\delta x^3) \simeq O\left(\frac{1}{M^2}\right)$$

Go to higher dimensions (D) $\qquad M = \frac{V}{(\delta x)^D}$

$$I_M - I = \left(\sum_i f(\vec{x}_i)(\delta x)^D - \int_{(\delta x)^D} d^D x \; f(\vec{x}) \right)$$



$$\int d^D x \left[f(\vec{x}_i) + \vec{\nabla} f(\vec{x}_i) \cdot \underbrace{(\vec{x} - \vec{x}_i)}_{\ell} + \dots \right]$$

$$(\delta x)^{D+1}$$

$$= O\left(M (\delta x)^{D+1} \right) \qquad (\delta x)^D = \frac{V}{M}$$

$$= O\left(M \left(\frac{V}{M}\right)^{1+\frac{1}{D}} \right) = O\left(\frac{1}{M^{1/D}} \right)$$

$$I = \int_V d^D x \; f(\vec{x})$$

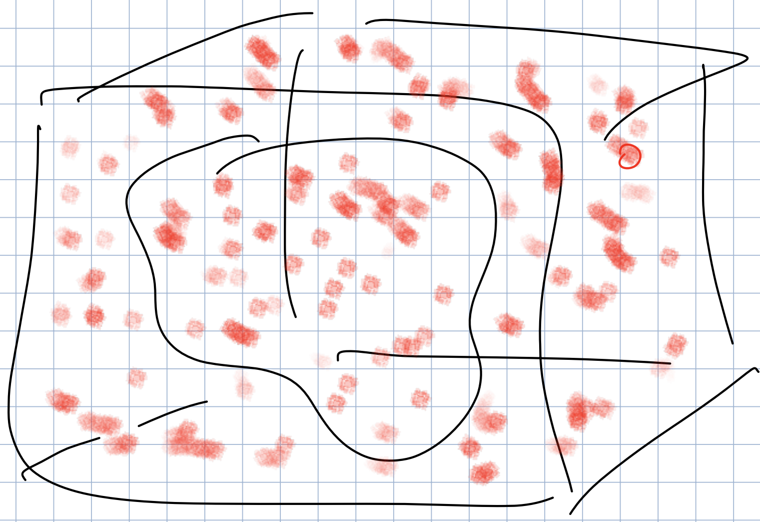
Reconsider random sampling

$$\varepsilon = | I_M - I | \sim O\left(\frac{1}{\sqrt{M}} \right)$$

M necessary to achieve a precision of ε

$$M \simeq \frac{A}{\varepsilon^2}$$

How is A behaving with D?



Statistical physics : Ising model

N Ising spins

$$I = \langle O(\vec{\sigma}) \rangle = \sum_{\vec{\sigma}} O(\vec{\sigma})\, p(\vec{\sigma})$$

$$p(\vec{\sigma}) = \frac{e^{-\beta H(\vec{\sigma})}}{Z}$$

entropy $\quad S = k_B \log \Omega_{eff}$

Ω_{eff} is the effective # of configurations that contribute to I

$$= e^{S/k_B} \qquad S = N s$$

$$\Omega = 2^N = e^{N \log 2}$$

$$\frac{\Omega_{eff}}{\Omega} = e^{N\left(\frac{s}{k_B} - \log 2\right)} \sim O(\exp(-\alpha N)) \qquad \frac{s}{k_B} < \log 2$$

$$\left(\frac{s}{k_B} - \log 2\right) < 0$$

Random sampling → importance sampling

$$I = \frac{1}{V}\int d^D x \; f(\vec{x})$$

So far $= \int d^D x \; f(\vec{x}) \; \tilde{p}(\vec{x})$ $\qquad \tilde{p}(\vec{x}) = \frac{1}{V}$

generalize:

$$= \int d^D x \; \overbrace{\left(\frac{f(\vec{x})}{p(\vec{x})}\right)}^{g(\vec{x})} \; \frac{p(\vec{x})}{V}$$

$\frac{p(\vec{x})}{N}$ normalized

$$= \frac{N}{V} \int d^D x \; g(\vec{x}) \; \frac{p(\vec{x})}{N} = \frac{N}{V} \langle g \rangle_{p/N}$$

How do I choose p ?

choose p so as to select the "support" of f

$g = x(\,)$

How do we generate points $\vec{x}_i$ distributed according to $p(\vec{x})/N$?

meaning : $\boxed{\vec{x}_1, \vec{x}_2, \vec{x}_3, \ldots, \vec{x}_M}$:

$$\frac{n(\vec{x}_i)}{M} \underset{M\to\infty}{\simeq} \frac{p(\vec{x}_i)}{N} (\delta x)^D$$

$$\int_V \frac{p(\vec{x})}{N} d^D x = 1$$

if I manage to do this

$$I_M = \frac{1}{M} \sum_{k=1}^{M} g(\vec{x}_k) \underset{M\to\infty}{\simeq} I$$

Rejection Monte Carlo

→ extract $\vec{x}$ at random in V

→ calculate $P = \frac{p(\vec{x})}{N} (\delta x)^D \in [0, 1]$

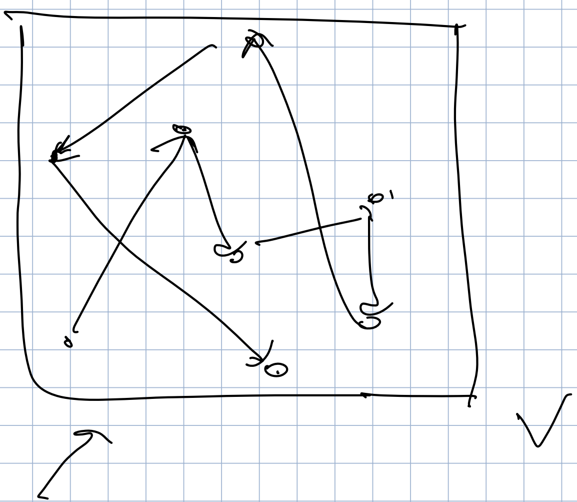
→ extract a random number $z \in [0, 1]$

→ if $z \leq P$ then $\vec{x} = \vec{x}_k$

$(k = 1, 2, \ldots, M)$

→ otherwise I reject $\vec{x}$

Markov-Chain Monte Carlo (MCMC)

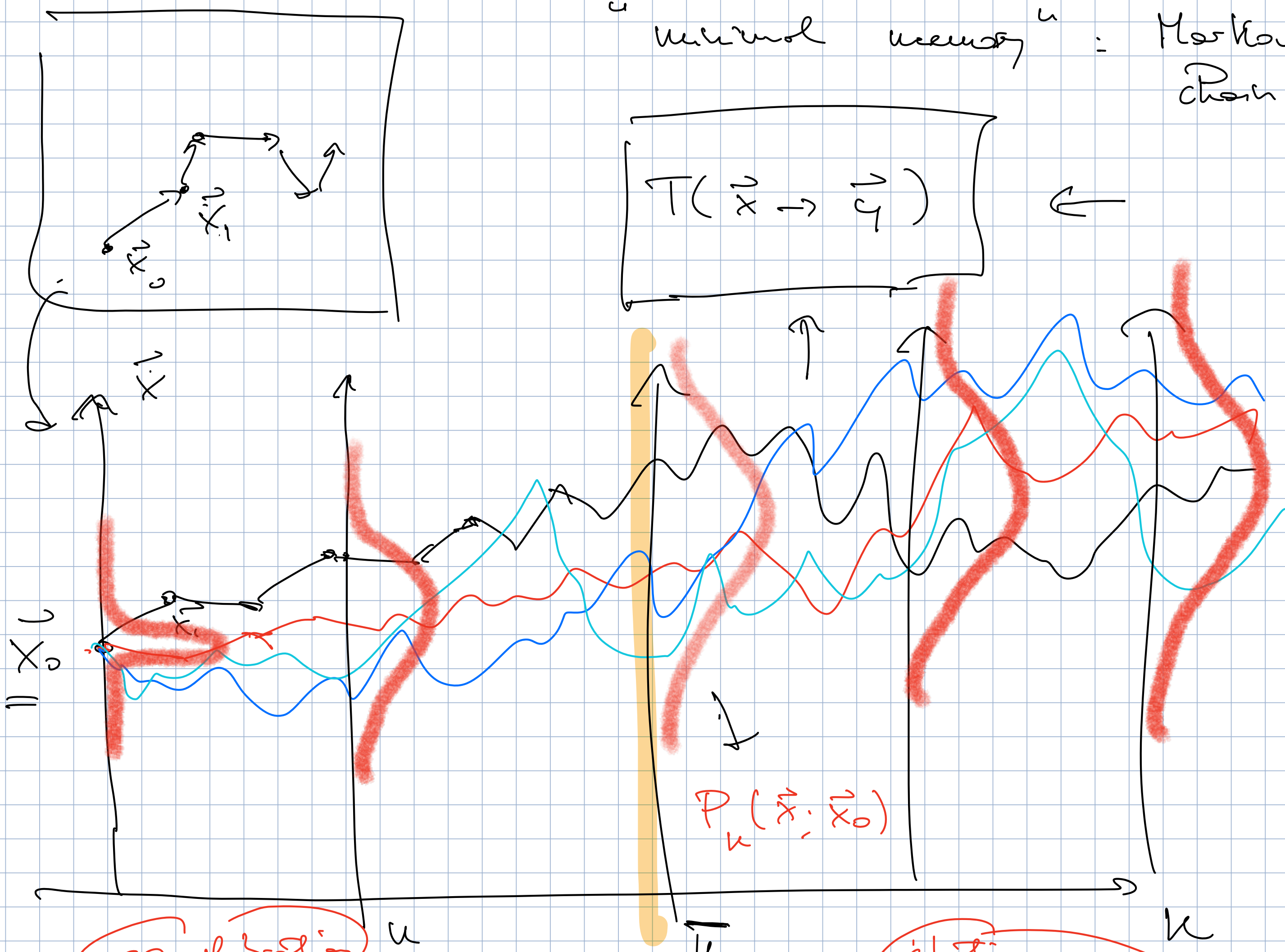


random sampling: no memory of previous actions

MCMC

"minimal memory": Markov Chain

$T(\vec{x} \to \vec{y})$



$$P_k(\vec{x}; \vec{x}_0) \xrightarrow{k \gg \bar{k}} P(\vec{x})$$

goal : $$\boxed{P(\vec{x}) = \frac{p(\vec{x})}{N}}$$

Condition on $T(\vec{x} \to \vec{y})$

transition probability