Numerical integration : Monte-Carlo method

multi-dimensional integrals

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

D-dimensional space

$D \gg 1$

$$\vec{x} = (x_1, \dots, x_D)$$

Ex. Statistical physics

ensemble of N particles in 3d

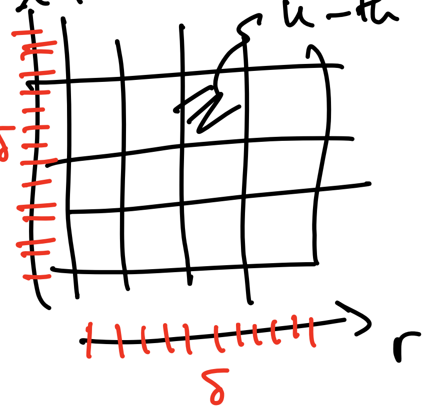
$\rightarrow \{\vec{r}_i, \vec{p}_i\} = \vec{x}$ $\qquad D = 6N$

$3N + 3N$ position & momenta ("phase space")

$$I = \langle O(\{\vec{r}_i, \vec{p}_i\}) \rangle_{T,N,V} = \frac{\int \prod_{i=1}^{N} d^3 r_i \, d^3 p_i \; O(\{\vec{r}_i, \vec{p}_i\}) \, e^{-\beta H}}{\int \prod_i d^3 r_i \, d^3 p_i \; e^{-\beta H}}$$

$$H = H(\{\vec{r}_i, \vec{p}_i\})$$

$$\beta = \frac{1}{k_B T}$$



$$\simeq \frac{\sum_{k=1}^{P} O(\{\vec r_i^{(k)}, \vec p_i^{(k)}\})\, e^{-\beta H(\{\vec r_i^{(k)}, \vec p_i^{(k)}\})}}{\sum_k e^{-\beta H}}$$

$P(\vec x)$

$$P = \frac{V}{\delta^{6N}} = V e^{(-\log\delta)N} \sim O(\exp(N))$$

$$\delta^{-6N} \qquad (\log\delta < 0)$$

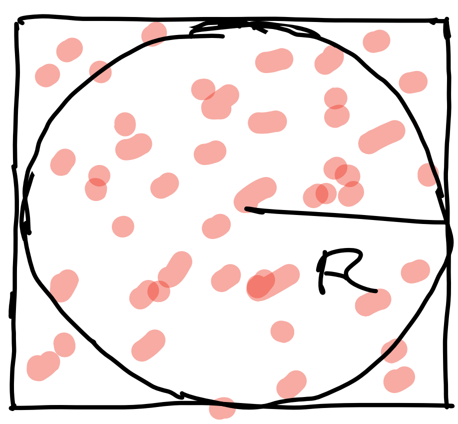
STRATEGY:

Estimate I with some finite precision using random numbers

"stochastic methods"

Estimating π

3,1416....



$$A_\circ = \pi R^2$$

$$A_\square = 4R^2$$

$$4\frac{A_\circ}{A_\square} = \pi$$

$$4\frac{N_\circ}{N_\square} \overset{N_\square\to\infty}{\simeq} \pi \quad \leftarrow$$

$$p = \frac{A_{\odot}}{A_{\square}}$$

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

M → tot. # of drops

m ← # of drops in $\odot$

$$\langle m \rangle_p = pM$$

$$\sigma^2_{m/M} = \frac{\langle m^2 \rangle_p}{M^2} - \frac{\langle m \rangle^2_p}{M^2} = M \frac{p(1-p)}{M^2}$$

$$p \rightarrow \frac{m}{M} = \frac{N_{\odot}}{N_{\square}}$$

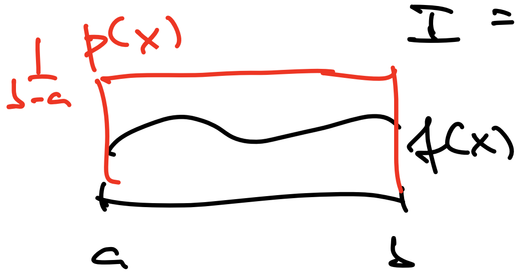
$$\sigma^2_{m/M} = \frac{\sigma^2_m}{M^2} = \frac{p(1-p)}{M}$$

$$\rightarrow \sigma_{m/M} \simeq \sqrt{\frac{p(1-p)}{M}} \sim O\left(\frac{1}{\sqrt{M}}\right)$$

$$\pi \pm \epsilon \qquad M \sim \frac{1}{\epsilon^2}$$

Random sampling for numerical integration

one-dimensional integral



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

$$= \int_a^b dx\, p(x)\, f(x) = \langle f \rangle_p$$

$$p(x) = \frac{1}{b-a}$$

generate a sample $x_1, x_2, x_3, \ldots, x_M$

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

if $\{x_i\}$ is generated according to $p(x)$

$|I_M - I|$ How does it depend on M?

x_i : are equally distributed independent random variables $(p(x))$

$f(x_i)$ " "

I_M = sum of random variables

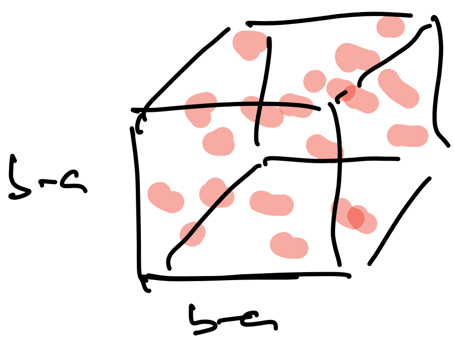
central limit theorem

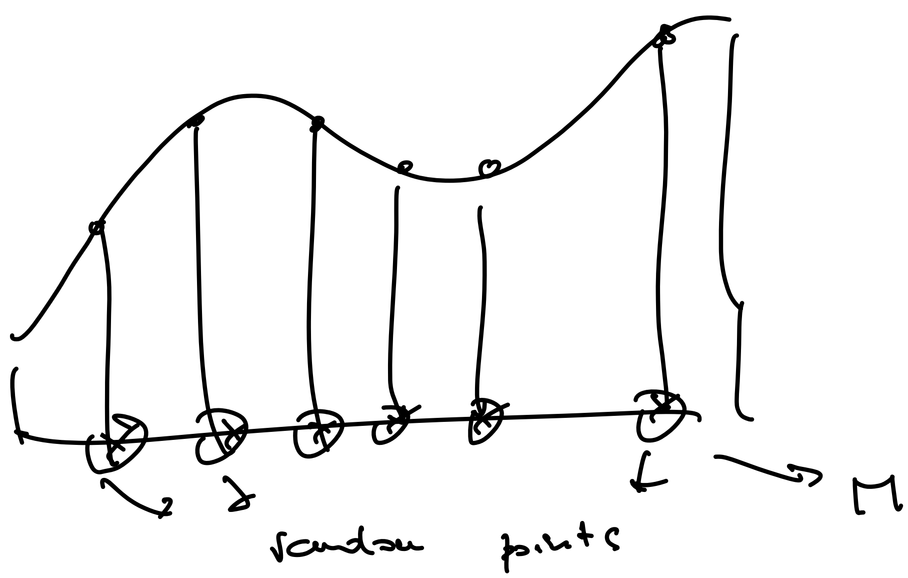
σ_f^2 is the variance of $f(x_i) = f_i$

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

$$\overline{I_M} = I = \frac{1}{M}\sum_{i=1}^{M} \overline{f}$$

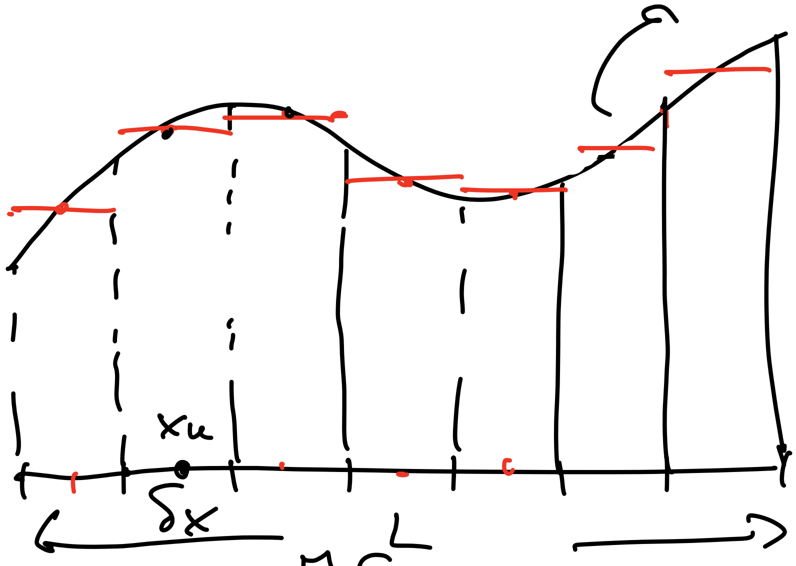
$$|I_M - I| \sim \sigma_{I_M} \sim O\left(\frac{1}{\sqrt{M}}\right)$$





random sampling

mid-point method



$$I_M - I = \sum_{n=1}^{M} \left[\delta x \, f(x_n) - \int_{x_n-\delta x/2}^{x_n+\delta x/2} dx \, f(x) \right]$$

$$= \sum_{n}^{M} \left[\delta x \, \cancel{f(x_n)} - \cancel{f(x_n)} \, \delta x \right.$$

$$- \cancel{\int_{x_n-\delta x/2}^{x_n+\delta x/2} dx \, f'(x_n)(x-x_n)}$$

$$\left. - \frac{1}{2} \int dx \, f''(x_n) (x-x_n)^2 + \dots \right.$$

$$\mathcal{O}(\delta x^3)$$

$$\sim \mathcal{O}(M (\delta x)^3) \sim \mathcal{O}\left(\frac{1}{M^2}\right)$$

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

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

$$I_M - I \simeq \sum_{k=1}^{M} \left[f(\vec{x}_k)(\delta x)^D - \int_{V_k} d^D x \, f(\vec{x}) \right]$$

$$= \sum_{k}^{M} \left[\cancel{f(\vec{x}_k)(\delta x)^D} - \cancel{f(\vec{x}_k)(\delta x)^D} - \underbrace{\int_{V_k} \vec{\nabla} f(\vec{x}_k) \cdot (\vec{x} - \vec{x}_k)\, d^D x}_{O(\delta x)^{D+k}} + \ldots \right]$$

$$k \geq 1$$

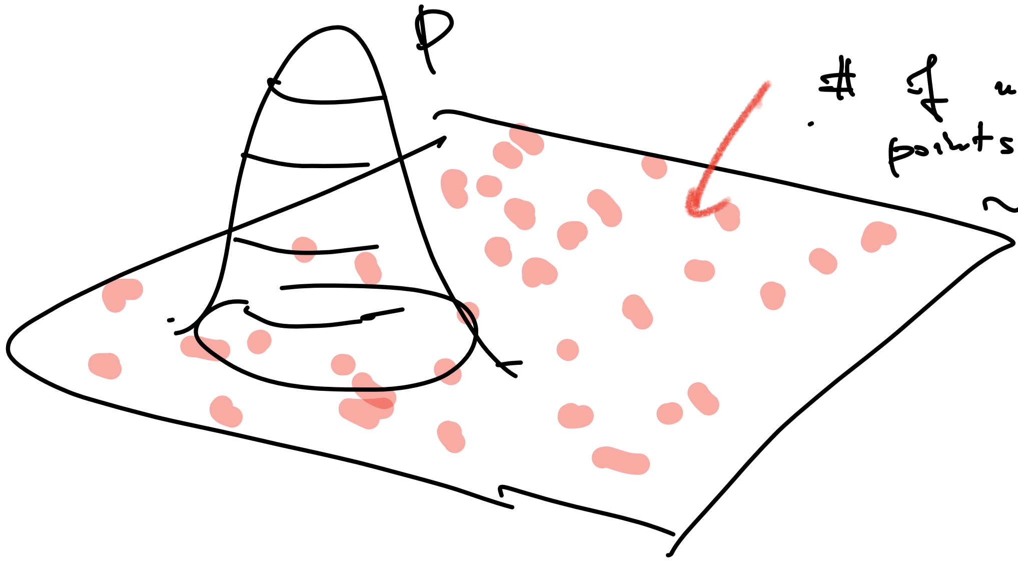
$$(\delta x)^D = \frac{V}{M} \qquad \delta x = \left(\frac{V}{M}\right)^{1/D}$$

$$I_M - I \sim M \, O\left(\frac{1}{M^{1+\frac{k}{D}}}\right) = O\left(\frac{1}{M^{k/D}}\right)$$

$\underline{D \gg 1}$ if $\frac{k}{D} < \frac{1}{2}$

<u>random sampling wins?</u>

Random sampling $\quad |I_M - I| \sim O\left(\frac{1}{\sqrt{M}}\right)$



\# of useless points $\sim O(\exp(D))$

a way not to waste too many points :
generate them with "importance sampling"

Need to have a clever distribution $p(\vec{x})$ (not flat)

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

$$= \int d^D x \left[\frac{1}{V}\frac{f(\vec{x})}{p(\vec{x})}\right] p(\vec{x})$$

$g(\vec{x})$

($p(\vec{x})$ is normalized)

$$= \langle g \rangle_p$$

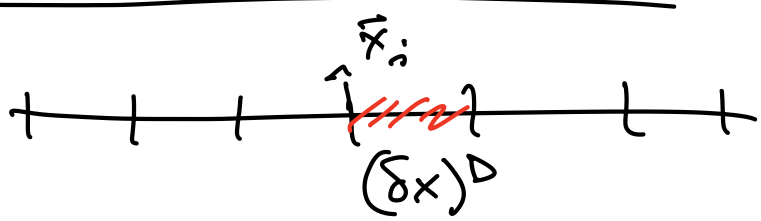
p is chosen so as to have significant weight where f has significant weight

Generate points $\vec{x}_n$ distributed according to $p(\vec{x})$

$$\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \dots, \vec{x}_M$$

# of times that $\vec{x}_n$ appears in the sequence is $\sim p(\vec{x}_n)$

"Rejection Monte Carlo"



1) draw $\vec{x}_i$ at random

2) $p(\vec{x}_i)(\delta x)^D = P_0$

3) draw a random number $z \in [0,1]$

4) if $z < P_0$ $\rightarrow$ accept the point in the sample

otherwise do nothing

after some time: M successful extractions

$\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_M$

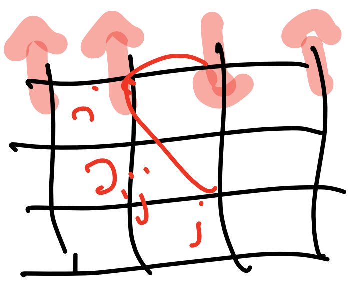
Think about a statistical sums for simple variable

$$\vec{x} \to \vec{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_D)$$

$(x_1, x_2, \ldots, x_D)$ $\qquad \sigma_i = \pm 1$ Ising variable

$$\langle O(\vec{\sigma}) \rangle = \frac{\sum_{\vec{\sigma}} O(\vec{\sigma})\, e^{-\beta H(\vec{\sigma})}}{\sum_{\vec{\sigma}} e^{-\beta H(\vec{\sigma})}} \qquad p(\vec{\sigma})$$

$$H(\vec{\sigma}) = -\sum_{ij} J_{ij} \sigma_i \sigma_j \qquad \text{Ising model}$$



\# of Ising configurations $\qquad 2^D$

$=$

$$\Omega \simeq e^{S}$$

$=$

$S \simeq \log \Omega$ $\qquad\qquad$ $S \leq D \log 2$

$$\frac{\Omega}{2^D} = \frac{e^{S}}{e^{D \log 2}} = e^{(S - D\log 2)} = e^{D\left(\frac{S}{D} - \log 2\right)}$$

<0

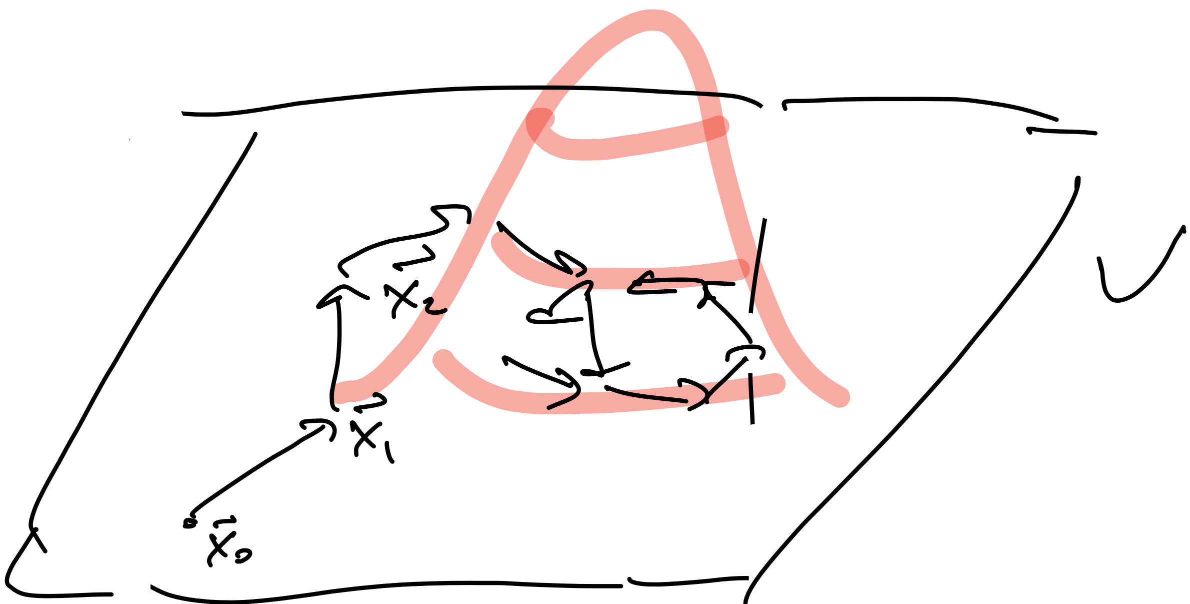
$\sim o(\exp(-D))$

"curse of dimensionality"

<u>Markov-Chain Monte Carlo</u>

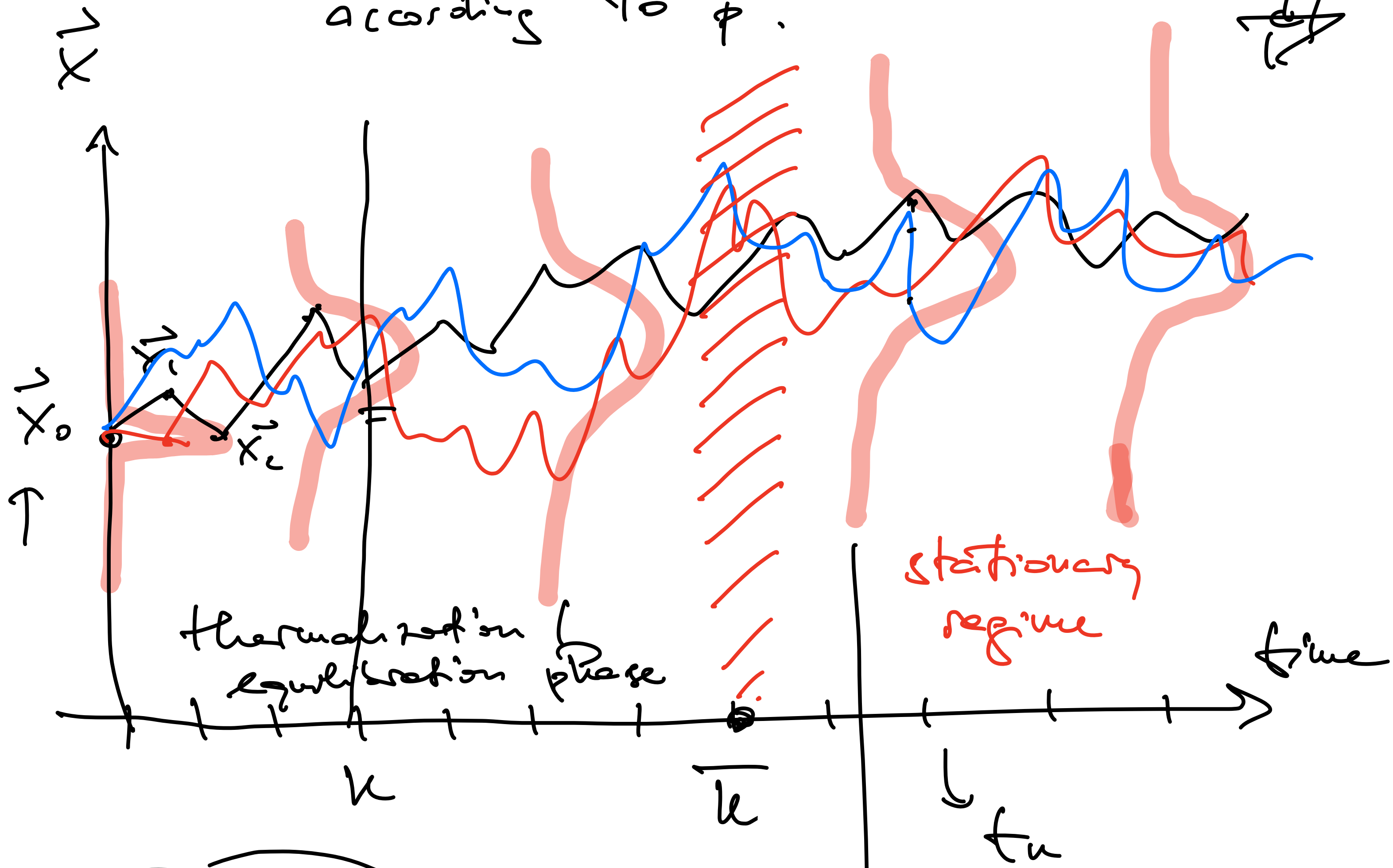
$\downarrow$

random walk



Markov chain : $T(\vec{x} \to \vec{y})$ transition probability

Idea: you choose T such that, (after some time) points $\vec{x}_n$ in the random walk are distributed according to p.



$$P_n(\vec{x}; \vec{x}_0, T)$$

$$P_k(\vec{x}; \vec{x}_0, T) \equiv P(\vec{x})$$

$$p(\vec{x})$$

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

$$\frac{dP_u}{dt} = P_{u+1}(\vec{x};\vec{x}_0) - P_u(\vec{x};\vec{x}_0)$$

$$= \sum_{\vec{y}} \underbrace{\left[P_u(\vec{y};\vec{x}_0)\, T(\vec{y}\to\vec{x})\right]}_{T} - P_u(\vec{x};\vec{x}_0)\, T(\vec{x}\to\vec{y}) \Big]$$

$$= 0$$

$$\sum_{\vec{y}} \left[\underbrace{p(\vec{y})\, T(\vec{y}\to\vec{x})} - \underbrace{p(\vec{x})\, T(\vec{x}\to\vec{y})}_{=0} \right]$$

detailed balance condition (on T)

$$p(\vec{y})\, T(\vec{y}\to\vec{x}) = p(\vec{x})\, T(\vec{x}\to\vec{y})$$

$$T(\vec{x}\to\vec{y}) = T_{prop}(\vec{x}\to\vec{y})\, \underbrace{A(\vec{x}\to\vec{y})}$$

proposal probability

acceptance probability

$$A(\vec{x} \to \vec{y}) = \underbrace{\frac{T_{prop}(\vec{y} \to \vec{x})}{T_{prop}(\vec{x} \to \vec{y})}}_{=1} \frac{p(\vec{y})}{p(\vec{x})} A(\vec{y} \to \vec{x})$$

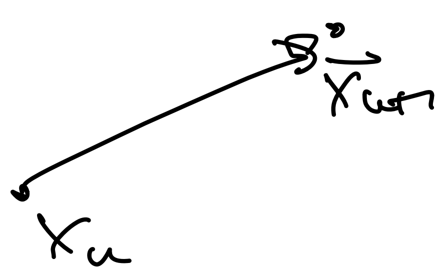
Symmetric proposal probabilities

$$A(\vec{x} \to \vec{y}) = \frac{p(\vec{y})}{p(\vec{x})} A(\vec{y} \to \vec{x})$$

$$=$$

Metropolis - Hastings solution

$$A(\vec{x} \to \vec{y}) = \min\left(1, \frac{p(\vec{y})}{p(\vec{x})}\right)$$



extract $\vec{y}$ according to $T_{prop}(\vec{x} \to \vec{y})$

extract $z \in [0, 1]$

if $z < \min\left(1, \frac{p(\vec{y})}{p(\vec{x})}\right)$

$\Rightarrow \vec{x}_{u+1} = \vec{y}$

otherwise $\vec{x}_{u+1} = \vec{x}_u$