12. Monte Carlos Methods

(method)

MC - Integration

use random numbers to approximate integrals

(physics)

MC - simulation

compute thermodynamic averages (next week)

12.1. MC - Integration

Write integral $I = \int d\vec{x}\, g(\vec{x}) = \int d\vec{x}\, p(\vec{x}) f(\vec{x}) = \langle f \rangle_p$ as average of observable $f(\vec{x})$ with probability distribution $p(\vec{x})$

Example: compute area of unit circle

1.) get N equally distributed points in $[-1,1]^2$

2.) if the point (x,y) $x^2+y^2<1$ holds, we are in the circle (success)

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

3.) N_o successes from N samples are binomial distributed with

$$p(N_o) = \binom{N}{N_o} p^{N_o} (1-p)^{N-N_o} \quad \& \quad \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

$\rightsquigarrow$ average $$\langle N_o \rangle = \sum_{N_o=0}^{N} N_o\, p(N_o) = N \cdot p = N \cdot \frac{P}{4}$$

variance $$\sigma_{N_o}^2 = \langle (N_o - \langle N_o \rangle)^2 \rangle = N p (p-1)$$

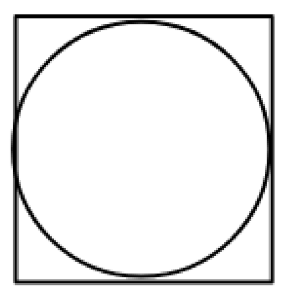
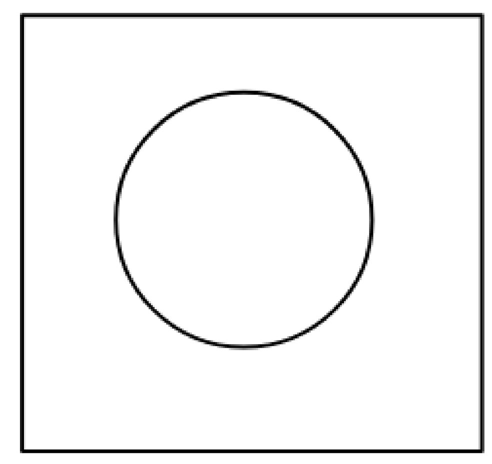
4.) therefore we conclude:

$$\boxed{\pi = A_\circ \approx \frac{N_\circ}{N} A_\square}$$

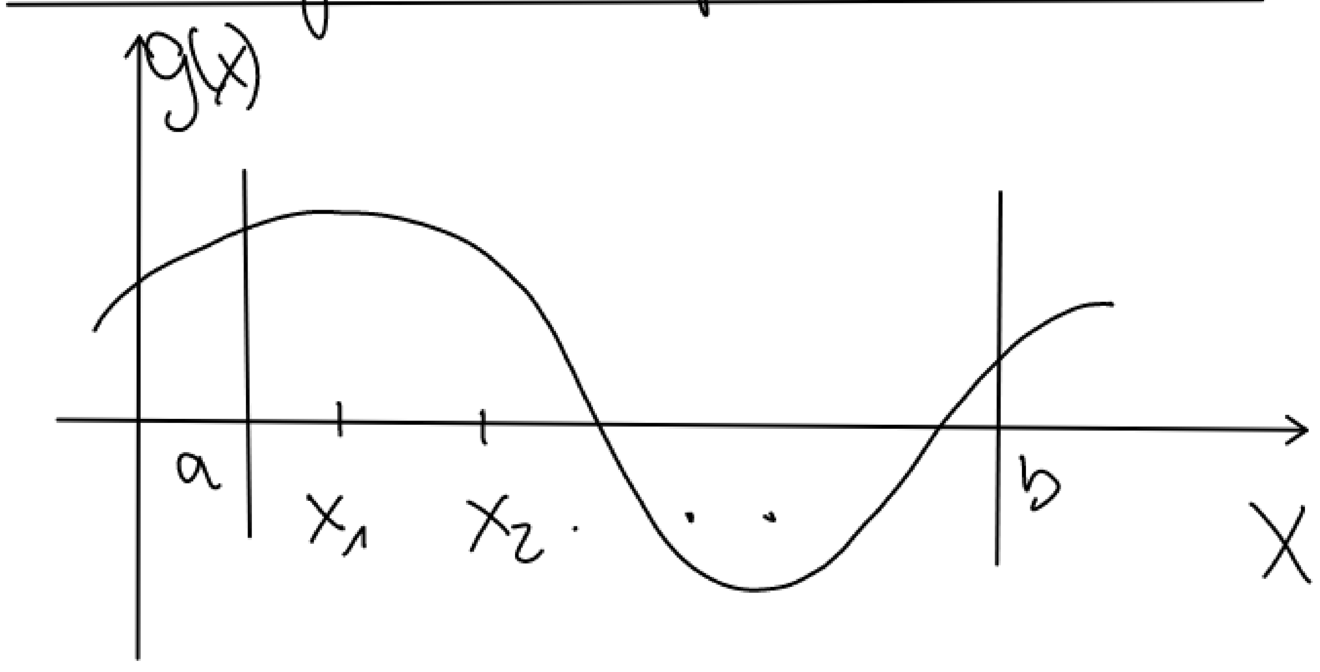
(statistical) error from variance

$$\sigma^2_{A_\circ} = \frac{A_\square^2}{N^2}\,\sigma^2_{N_\circ} = \frac{1}{N} A_\circ (A_\square - A_\circ) \sim \frac{1}{N}$$

$\rightsquigarrow$ error $\sim 1/\sqrt{N}$ best when $A_\square - A_\circ$ small

i.e.  instead of 

For general function



choose N random

$x_i \in [a,b]$

avg. dist. between points

$$\boxed{I_{MC} = \frac{b-a}{N} \sum_{i=1}^{N} g(x_i)}$$

distribution $p(x) = \begin{cases} \frac{1}{b-a} & \text{for } x \in [a,b] \\ 0 & \text{otherwise} \end{cases}$

$$I = \int_a^b dx\, g(x) = \int dx\; p(x) \underbrace{(b-a)\, g(x)}_{f(x)} = \langle f \rangle_p$$

$$= \langle f \rangle_p \approx \frac{1}{N} \overbrace{\sum_{i=1}^{N} f(x_i)}^{y} = \frac{b-a}{N} \sum_{i=1}^{N} g(x_i) = I_{MC}$$

error from variance σ_I^2 Gauß distributed

central limit theorem: $\langle y \rangle = N \cdot \langle f \rangle$ and

$\sigma_y^2 = N \cdot \sigma_f^2 \sim \; = \langle f^2 \rangle - \langle f \rangle$

$$\rightsquigarrow \sigma_I^2 = \frac{1}{N^2} \sigma_y^2 = \frac{1}{N} \sigma_f^2 \sim \frac{1}{N} \rightsquigarrow \text{error} \sim \frac{1}{\sqrt{N}}$$

compare with sec. 3 trapezoid meth. $\sim N^{-2}$

Simpson –"– $\sim N^{-4}$:-(

advantage for $\boxed{\text{higher, } n \text{, dimensions}}$

MC $\sim N^{-1/2}$ trapezoid meth. $\sim N^{-2/n}$

simpson –"– $\sim N^{-4/n}$:-)

12.2. Markov-Sampling & Metropolis-algorithm

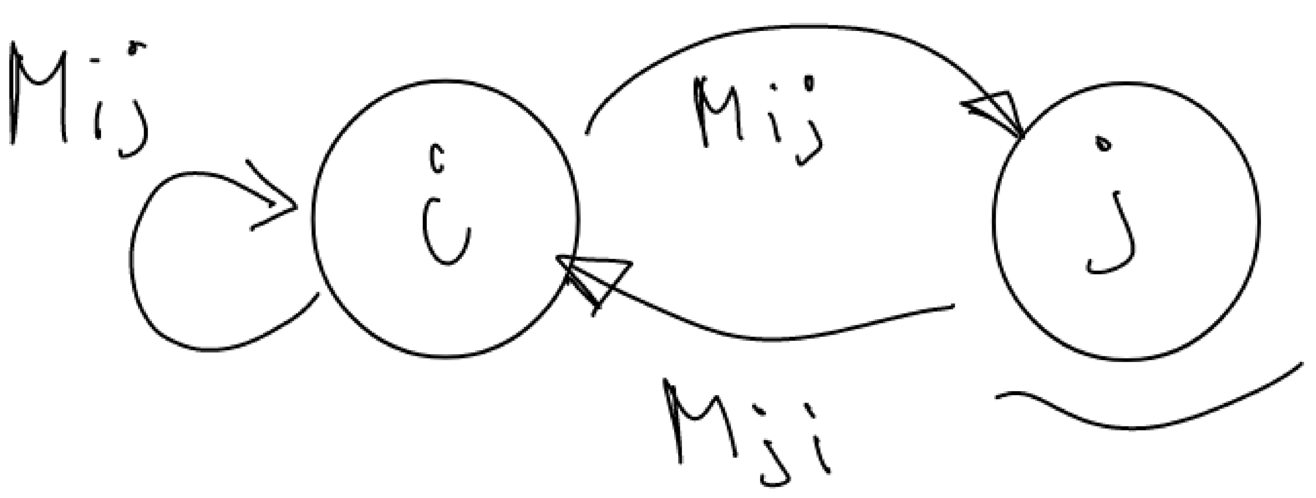
Question is there a better distribution $p(x)$?

Ideally $p(\vec{r}) = \begin{cases} c\,|g(\vec{r})| & \vec{r} \in V \\ 0 & \text{otherwise} \end{cases}$ with

$$1/c = \int_V d^n\vec{r}\,|g(\vec{r})| \quad \text{(importance sampling)}$$

- hard to compute c
- hard to generate random numbers for $p(x)$

Samples rather from dynamic random process,
<u>Markov-Process</u>



probabilities for state transitions only depend on the current state (no memory)

$$P_j(t+\Delta t) = \sum_i P_i(t)\, M_{ij} \quad \text{or} \quad \boxed{\begin{aligned} \vec{p}^{\,T}(t+\Delta t) &= \vec{p}^{\,T} M \\ \vec{p}^{\,T}(t+n\Delta t) &= \vec{p}^{\,T} M^n \end{aligned}}$$

with (i) $0 \le M_{ij} \le 1$, each is a probability

(ii) $\sum_j M_{ij} = 1 \iff \sum_i P_i = 1$

or $$P_i(t+\Delta t) - P_i(t) = \sum_j M_{ji} P_j(t) - \underbrace{\sum_j M_{ij}}_{1} P_i(t)$$

which can be written as

$$\boxed{\frac{P_i(t+\Delta t) - P_i(t)}{\Delta t} = - \sum_{j \neq i} J_{ij}}$$

continuity equation

current $$J_{ij} = \frac{1}{\Delta t}\left(- M_{ji} P_j + M_{ij} P_i\right) = - J_{ji}$$

requires $$\boxed{\frac{P_{eq,i}}{P_{eq,j}} = \frac{M_{ji}}{M_{ij}}}$$

next time

Metropolis-algorithm

to get such a process