# Numerical integration

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

$$\vec{x} = (x_1, x_2, \ldots, x_D)$$

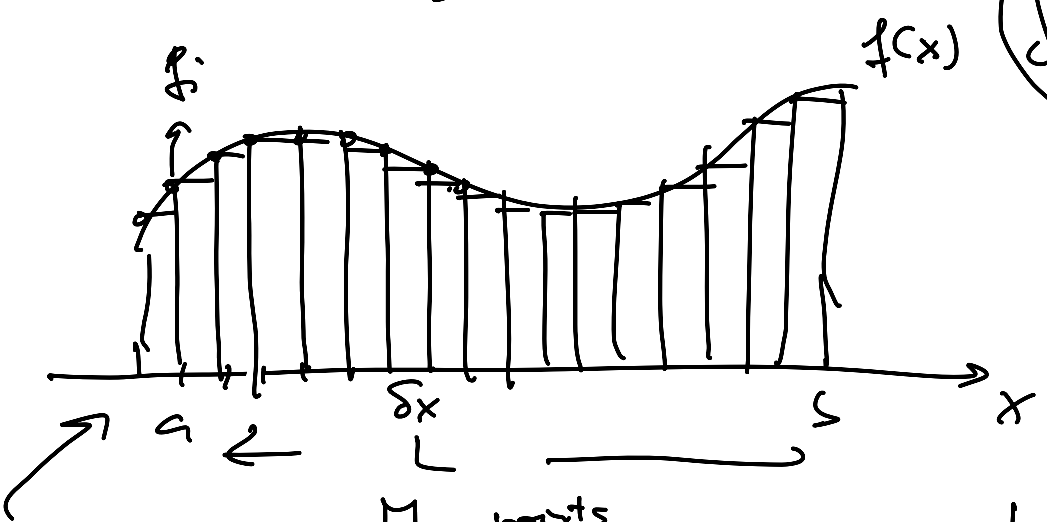
$$D \gg 1$$

$$\mathcal{H}(\{\vec{x}_i, \vec{p}_i\}) \qquad i = 1, \ldots, N$$

$$\langle O(\{\vec{x}_i, \vec{p}_i\}) \rangle = \frac{\int \left( \prod_{i=1}^{N} \frac{d^3 p_i \, d^3 x_i}{(2\pi\hbar)^{3N}} \right) O(\{\vec{x}_i, \vec{p}_i\}) \, e^{-\beta \mathcal{H}}}{\int \left( \prod_{i=1}^{N} \frac{d^3 p_i \, d^3 x_i}{(2\pi\hbar)^{3N}} \right) e^{-\beta \mathcal{H}}}$$

$$D = 6N$$

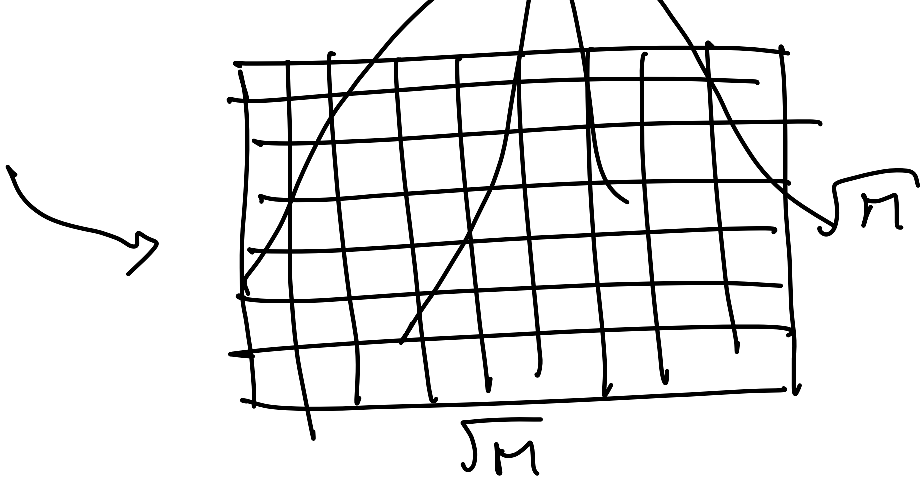
$$\int_a^b dx \; f(x) = I$$




$M$ points

$$L = M \delta x$$

$$I_M \simeq \sum_{i=1}^{M} f_i \, \delta x$$



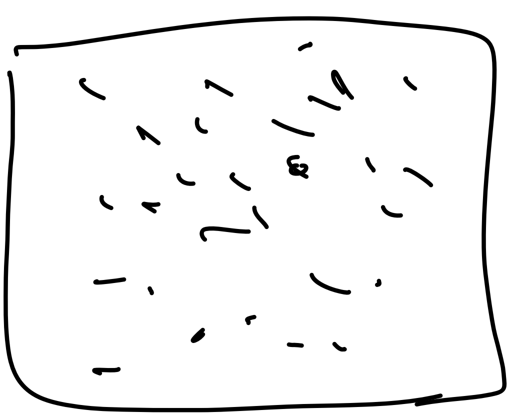
$$I_M \triangleq \sum_{i=1}^{M} f_i \, (\delta x)^2$$

D dimensional integral $\rightarrow$ $M^{1/D}$ points along each dimension

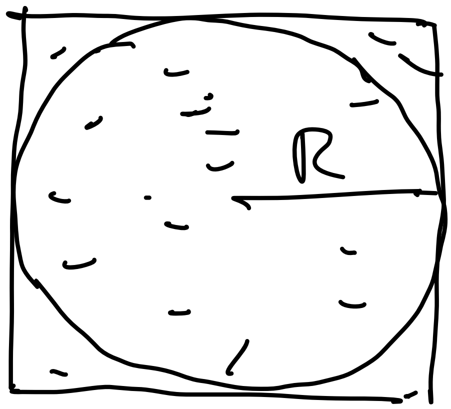
$M$ points along each dimension

$\rightarrow M^D \sim o(\exp(N))$

Monte Carlo methods: stochastic approach



$\{f_i\}$



$$A_{sq} = 4R^2$$

$$A_D = \pi R^2$$

$$4\frac{A_D}{A_{sq}} = \pi$$

$$P_D = \frac{\pi}{4}$$

$$4\frac{M_D}{M_{tot}} \underset{N_{tot}\to\infty}{\simeq} \pi$$

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

$$\frac{\langle m \rangle}{M} = p = \frac{\pi}{4}$$

$$\sigma_m^2 = \langle m^2 \rangle - \langle m \rangle^2 = M p (1-p)$$

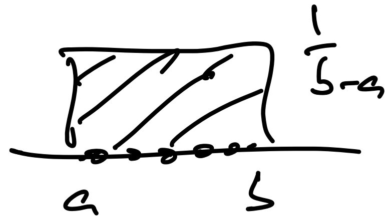
$$\frac{\sigma_m}{\langle m \rangle} = \frac{\sqrt{1-p}}{\sqrt{M}} \sim O\left(\frac{1}{\sqrt{M}}\right)$$

$$\to \epsilon \sim \frac{1}{\sqrt{M}} \qquad M_\epsilon \sim \frac{1}{\epsilon^2}$$

Evaluating integrals using random sampling

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

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




sampling points in $[a,b)$ according to $p(x)$

$$x_1,\ x_2, \dots,\ x_M$$
$$\downarrow$$
$$f_1 = f(x_1),\ f_2, \dots,\ f_M$$

$$\boxed{I_M = \frac{1}{M}\sum_{i=1}^{M} f(x_i)} \xrightarrow[M\to\infty]{} I$$

each point $x_i$ appears a number of times

$$n(x_i) : \quad \frac{n(x_i)}{M} \xrightarrow[M\to\infty]{} p(x_i)$$

$$\sum_k p(x_k)\, f(x_k)$$

sum of random variables
identically distributed

$$\boxed{\langle I_M \rangle = \frac{1}{M} \sum_{i=1}^{M} \langle f(x_i) \rangle_p} = I$$

$$\int dx\, p(x)\, f(x) = I$$

convergence $|I_M - I| \sim 0$ $\quad M \to \infty$ How ?

$f(x_i)$ random variable

$$\langle f \rangle = I$$

$$\langle f^2 \rangle = \int dx\, f^2(x)\, p(x)$$

$$\sigma_f^2 = \langle f^2 \rangle - \langle f \rangle^2$$

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

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

Central limit theorem

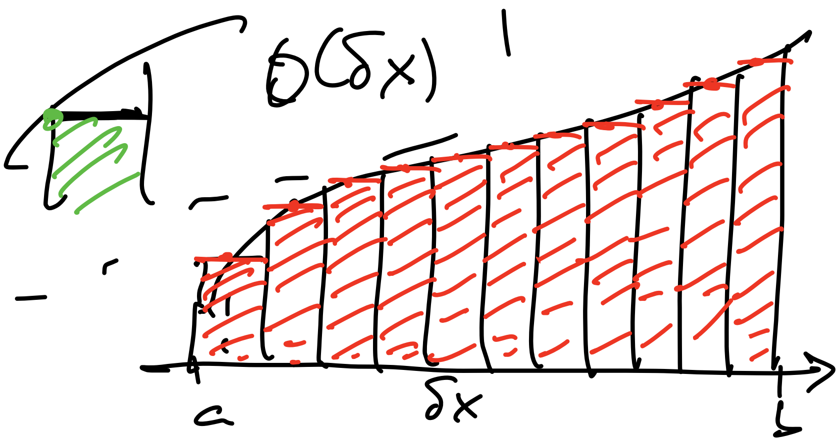
$$\boxed{|I - I_M| \simeq \sigma_{I_M} \sim O\left(\frac{1}{\sqrt{M}}\right)}$$

generalize the same calculation to

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

$$= \int_V d^D x \, p(\vec{x}) \, f(\vec{x})$$

**Deterministic integral evaluation** : can you do better than $\frac{1}{\sqrt{M}}$ ?




midpoint method

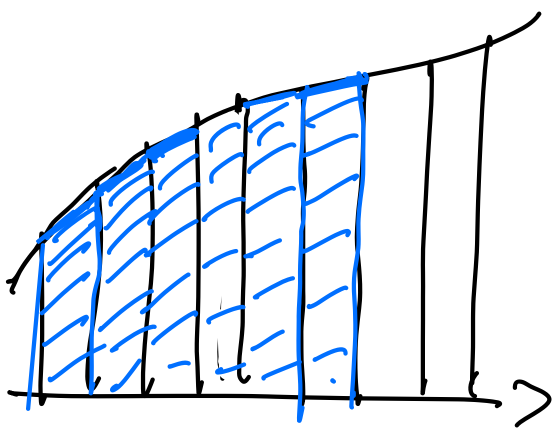
L M

error $O\left(\frac{1}{M^2}\right)$

↑

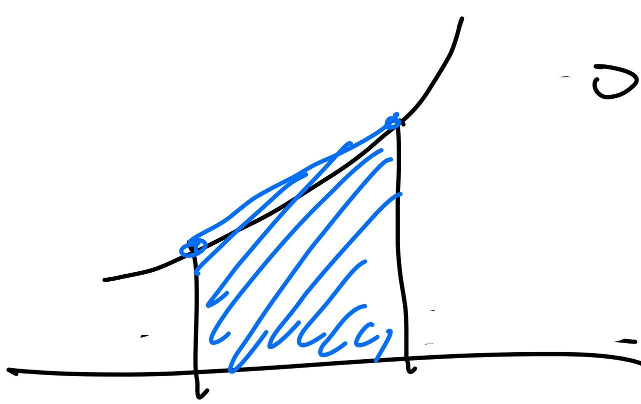
$O(\delta x^2)$

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



trapezoid method

$O\left(\frac{1}{M^3}\right)$



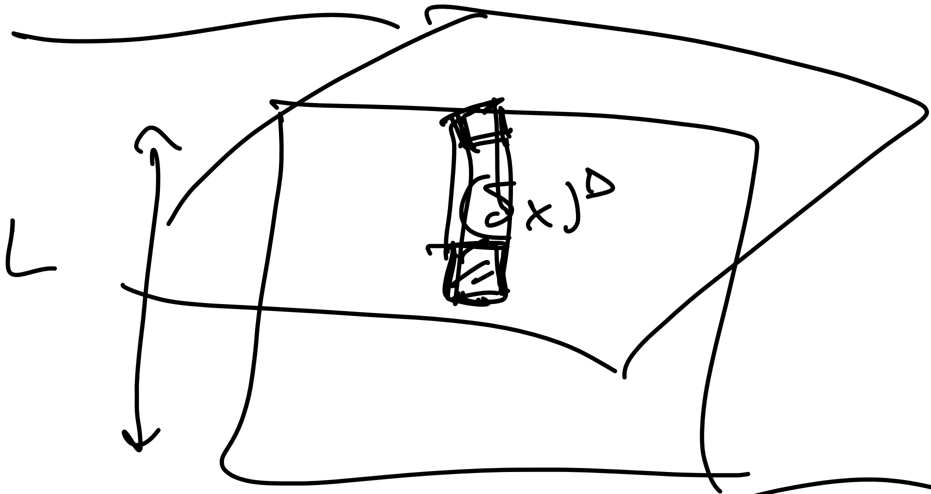
$O(\delta x^3)$

$1+2$

$O\left(\frac{1}{M^k}\right)$ deterministic methods

$k \geq 2$

M fixed $D > 1$




$\delta x = \frac{L}{M^{1/D}}$

error $O\left(M (\delta x)^{D+k}\right) \sim O\left(M \frac{L}{M^{1+k/D}}\right)$

error of the integral in of the cells

$\frac{L}{M^{\frac{1}{D}(D+k)}}$

$\sim O\left(\frac{1}{M^{k/D}}\right)$

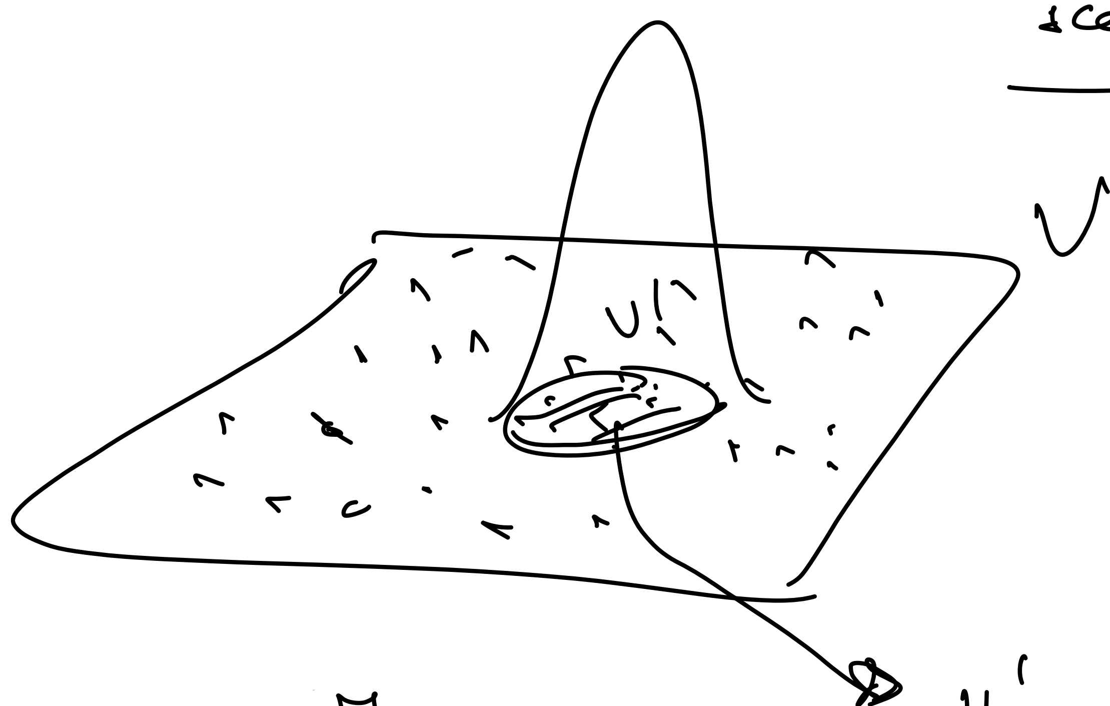
$\forall k$ if $D > 2k$ $\frac{k}{D} < \frac{1}{2}$

accuracy of $\epsilon$ ↓ $\qquad \epsilon \sim O\left(\frac{1}{\sqrt{M}}\right)$

$$M_\epsilon \simeq A_D \, \frac{1}{\epsilon^2}$$

$$A_D \sim O(\exp(D))$$

worst-case scenario




$$I_M = \frac{1}{M} \sum_{i=1}^{M} f(x_i) \qquad \frac{V'}{V} \sim O(\exp(-D))$$

ex. $$\langle O \rangle = \frac{\int \left( \prod_i d^3x_i \, d^3p_i \right) O \, e^{-\beta H}}{\int \left( \prod_i \right) e^{-\beta H}}$$

$$= \frac{\sum_c O_c e^{-\beta E_c}}{\sum_c e^{-\beta E_c}} \sim O(N)$$

$O(\exp(N))$

{ # of points $O(N \exp(-N))$ }

BADLY EXPRESSED! SEE NEXT LECTURE

Importance sampling

$$= \mathcal{N} \frac{\sum_c f_c p_c}{\sum_c p_c}$$

$$I = \mathcal{N} \frac{\int d^D x \, \frac{f(\vec{x})}{p(\vec{x})} p(\vec{x})}{\int d^D x \, p(\vec{x})} \qquad \frac{p(\vec{x})}{\mathcal{N}}$$

$g(\vec{x})$

$$\int d^D x \, p(\vec{x}) = \mathcal{N}$$

$$I = \int d^D x \, f(\vec{x})$$

extract points $\vec{x}_i$ with probability $p(\vec{x}_i)$

$\{ \vec{x}_i \} \qquad i = 1, \dots, M$

$$\frac{n(\vec{x}_i)}{M} \xrightarrow{M \to \infty} \frac{p(\vec{x}_i)}{\mathcal{N}}$$

goal

$$I_M = \frac{N}{M}\sum_{i=1}^{M} f(\vec{x}_i) \underset{M\to\infty}{\Longrightarrow} I$$

To build a sequence of points distributed according to $\frac{p(\vec{x}_i)}{N}$

## REJECTION MONTE CARLO

1) extract $\vec{x}_i$ at random
2) ev. $\frac{p(\vec{x}_i)}{N} = p_i$
3) extract $z \in [0,1]$

if $z \leq p_i$ $\rightarrow$ accept $\vec{x}_i$ into the pool (sample

$M \rightarrow M+1$

4) goto 1)

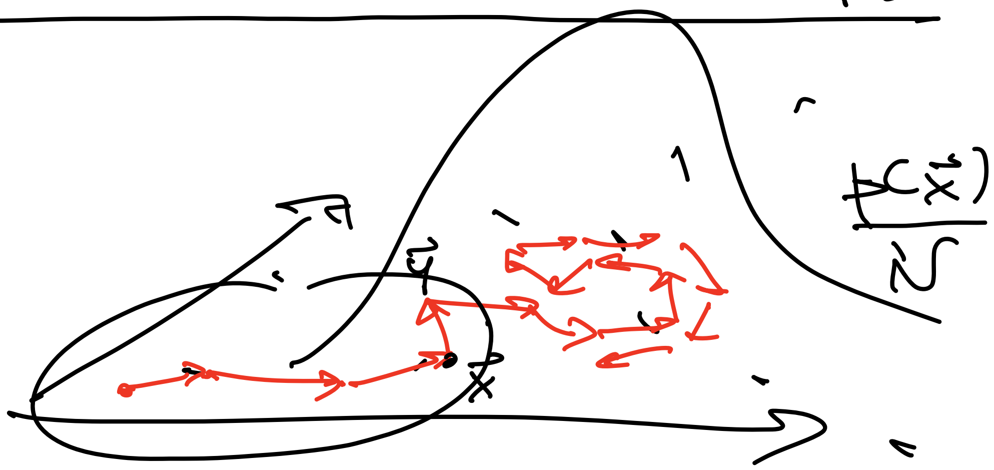
If you choose p selecting the important region of integration space for I

$\rightarrow$ throw away most of generated points

$\vec{x}_i$

Efficient approach to importance sampling

MARKOV-CHAIN MONTE CARLO




$\boxed{T(\vec{x} \to \vec{y})}$ transition probability