9.1. Monte-Carlo Integration

Expectation Value of $f(x)$ over PDF $p(x)$

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

[if const. PDF $p(x) = \frac{1}{b-a}$]

[$\langle f \rangle_p = \frac{1}{b-a}\int_a^b f(x)\,dx = J/_{b-a}$]

Squared Exp. Value (mean square, 2nd moment of PDF with f)

$$\langle f^2 \rangle_p = \int_a^b f^2(x)\,p(x)\,dx$$

[r.m.s. = root mean square $= \langle f^2 \rangle_p^{1/2}$]

$$\langle (f - \langle f \rangle_p)^2 \rangle_p = \int_a^b (\underline{\underline{f}} - \underline{\underline{\langle f \rangle_p}})^2\,p(x)\,dx = \underline{\langle f^2 \rangle_p} - \langle f \rangle_p^2 = \sigma^2 = Var(f)$$

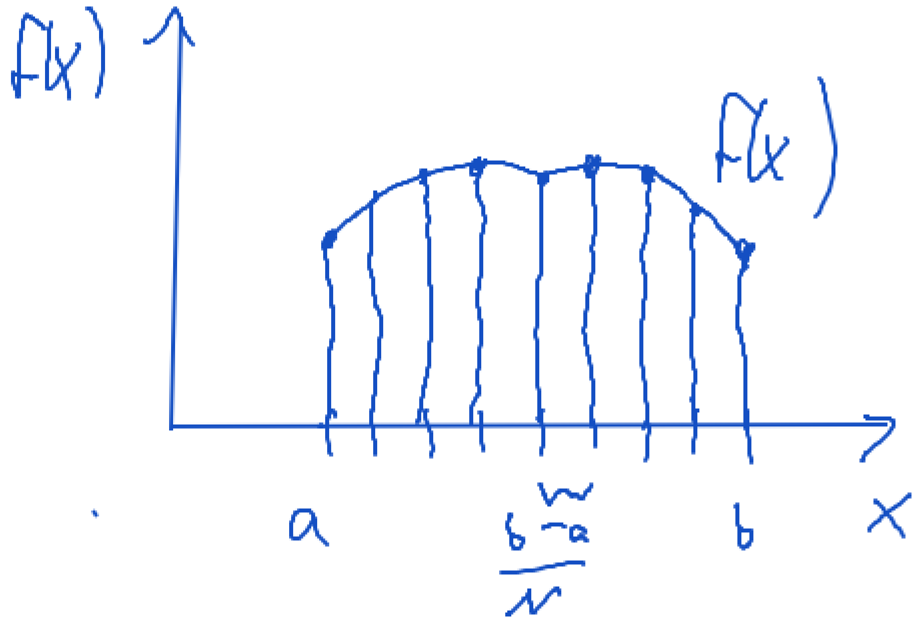
[r.m.s. deviation $= \langle (f - \langle f \rangle_p)^2 \rangle_p^{1/2} = \sigma$]

Empirical approximation of expectation value by a finite set of random numbers:

$$(*) \quad \overline{f_N} = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \qquad \text{using } x_i \text{ distr. acc. to } p(x)$$

$$(*) \quad \overline{f_N^2} = \frac{1}{N}\sum_{i=1}^{N} f^2(x_i) \; ; \quad \lim_{N\to\infty} \overline{f_N} = \langle f\rangle_p \; ; \quad \lim_{N\to\infty} \overline{f_N^2} = \langle f^2\rangle_p$$

In case of eq. distr. RN: $p(x) = \frac{1}{b-a}$



$$\langle f\rangle_p = \int f(x)\,p(x)\,dx = \frac{1}{b-a}\int_a^b f(x)\,dx = \frac{J}{b-a}$$

$$J = \int_a^b f(x)\,dx = (b-a)\cdot\langle f\rangle_p \overset{=}{=} \frac{(b-a)}{N}\sum_{i=1}^{N} f(x_i)$$

Repetition: $\langle (f - \langle f \rangle_p)^2 \rangle = \int_a^b (f - \langle f \rangle_p)^2 \, p(x)\, dx$

$$= \int_a^b \left(f^2 - 2 f \langle f \rangle_p + \langle f \rangle_p^2 \right) p(x)\, dx$$

$$= \int_a^b f^2(x)\, p(x)\, dx - 2 \langle f \rangle_p \int_a^b f(x)\, p(x)\, dx + \langle f \rangle_p^2 \underbrace{\int_a^b p(x)\, dx}_{=1}$$

$$= \langle f^2 \rangle_p - 2 \langle f \rangle_p \langle f \rangle_p + \langle f \rangle_p^2$$

$$= \langle f^2 \rangle_p - \langle f \rangle_p^2$$

$\overline{f_N}$: average of f (over ρ) over interval

$\overline{f_N^2}$: average of f^2

empirical mean and second moment

Approach 1: just make N very large to get good result

Approach 2: many „sweeps", many samples, use of „central limit theorem" (law of large numbers)

- We fix N to some intermediate value
- We compute $\overline{f_N}$ many times with that N, using different RN seeds. We get $\overline{f_{N,1}}$, $\overline{f_{N,2}}$, ... $\overline{f_{N,N_s}}$; N_s : sweeps

[Example: roll dice 10 times, $N=10$, take average $\overline{f_N}$; do this 10.000 times $N_s = 10.000$; look at the distribution of $\overline{f_N}$]

By "law of large numbers" (central limit theorem) CLT

we find that the $\overline{f}_N$ have a Gaussian distribution around the expectation value $\langle f \rangle_p$

Simple Demonstration of CLT:

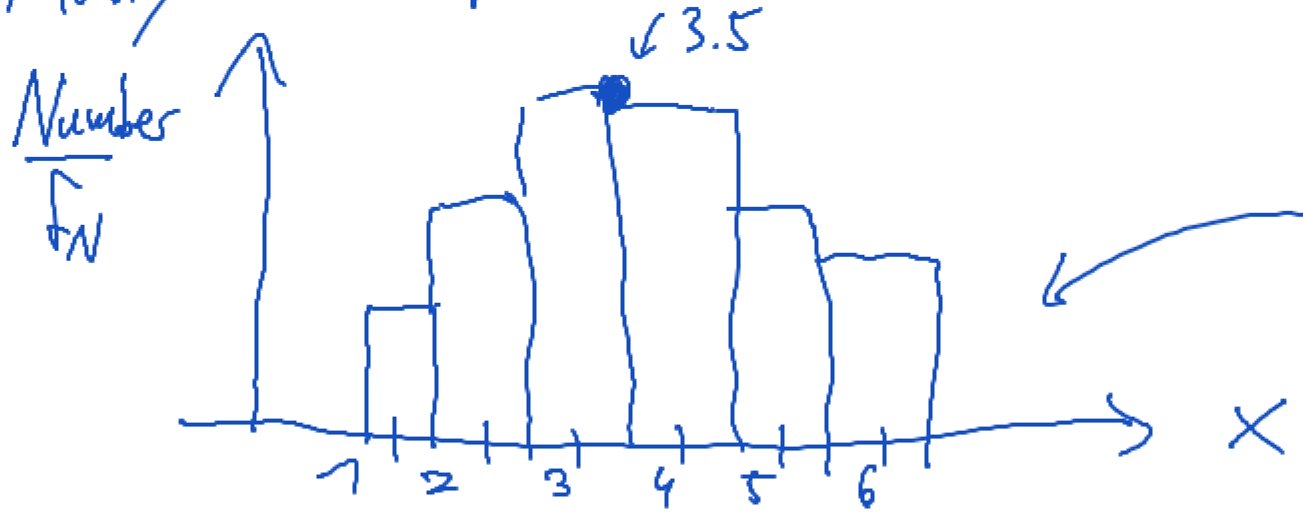
Rolling Dice: $\overline{f}_N = \frac{1}{N} \sum_{i=1}^{N} x_i$ $\quad 1 \le x_i \le 6$; x_i integer

One Sweep: N times rolling dice (Expectation value: $\langle f \rangle_p = 3.5$)

Many Sweeps: Distribution of $\overline{f}_N$; $N = 10$

$$10 \le \overline{f}_N \cdot N \le 60$$

$$1 \le \overline{f}_N \le 6$$



Gaussian distribution around the exp. value 3.5

CLT, cont'd: 1) $\overline{f_N}$ have Gaussian distribution around $\langle f \rangle_p$

2) Variance of distribution of $\overline{f_N}$ is σ_N:

$$\sigma_N^2 = \frac{1}{N-1}\left[\overline{f_N^2} - \overline{f_N}^2\right] \sim \frac{1}{N}\left[\underbrace{\langle f^2\rangle - \langle f\rangle^2}_{Var(f)}\right]$$

What we take from it? Compute $\overline{f_N}$, $\overline{f_N^2}$ many times

Gaussian

1/e

σ: FWHM

full width, half maximum

1/e

$$\sigma_N^2 = \frac{1}{N-1}\left[\overline{f_N^2} - \overline{f_N}^2\right]$$

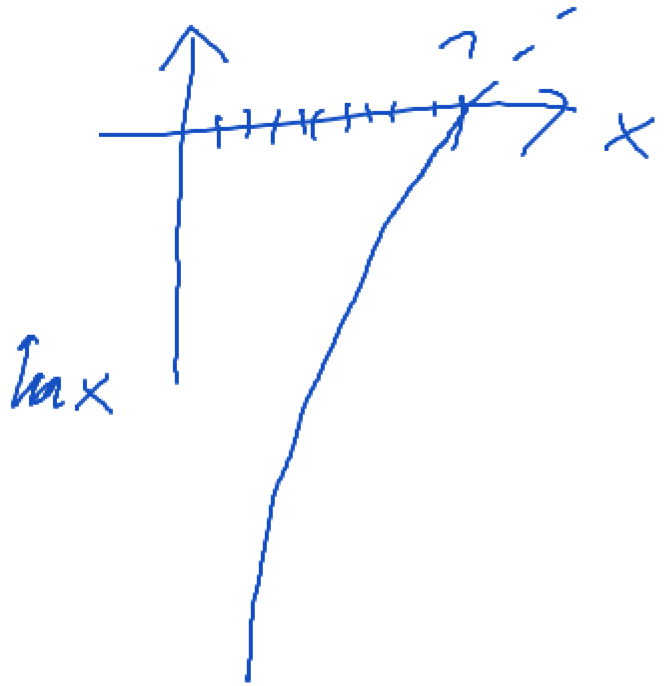
Importance Sampling / Metropolis Algorithm

Computing of the $\overline{f_N}$, $\overline{f_N^2}$ with special $p(x)$

$$\overline{f_N} = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \qquad \text{with } x_i \text{ distr. acc. to PDF } p(x)$$

If the function f is strongly varying in the definition set;

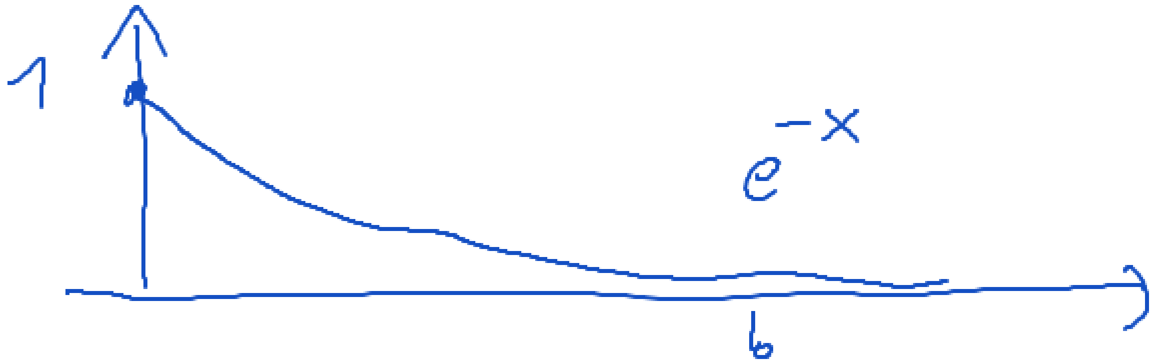
for ex. $f(x) = \ln x$; $\langle f \rangle_p = \int_\varepsilon^1 f(x)\,p(x)\,dx$ $\qquad \varepsilon > 0$



- Use $p(x)$ not equally distr.
- Importance Sampling

$f(x) = e^{-x}$; $f(x)$ is very small in large parts of definition set;

$0 \le x \le a \to \infty$



Importance Sampling: choose another function $g(x)$ „near" $f(x)$

$$I = \int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)}\, g(x)\,dx$$; choose RN's

with PDF $g(x)$; $1 = \int_a^b g(x)\,dx$

$$\overline{f_N} = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{g(x_i)}$$ with RN x_i distr. acc. to $g(x_i)$ approximates I

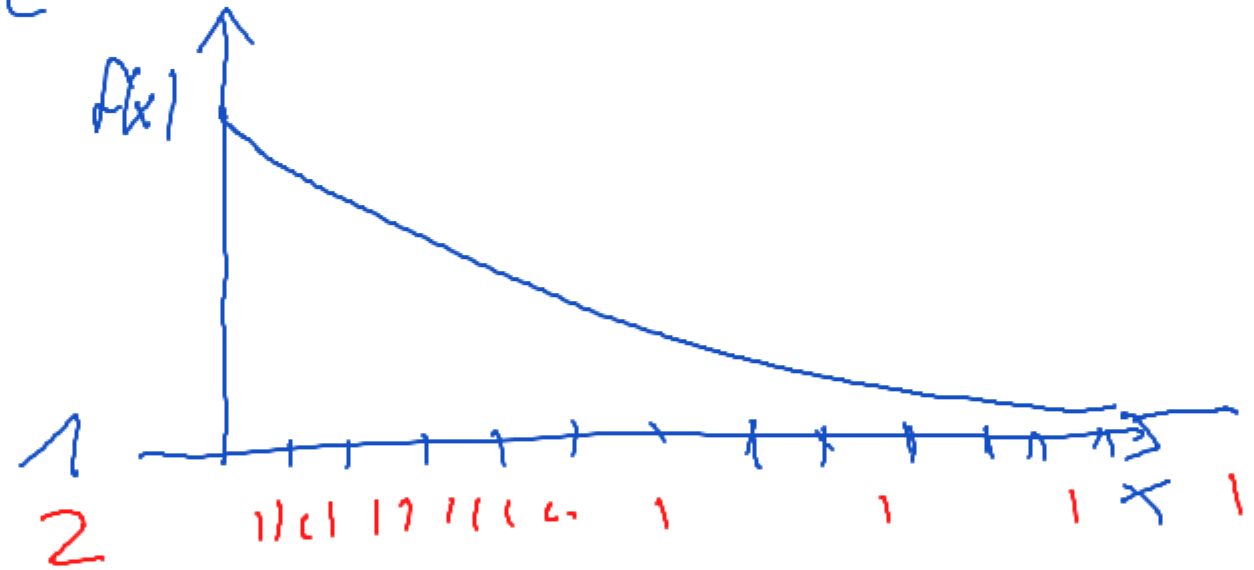
Application example: $f(x) = e^{-x}$; $I = \int_a^b f(x)\,dx$

Method 1: $\overline{f}_N = \frac{1}{N} \sum_{i=1}^{N} e^{-x_i}$ w. eq. distr. RN x_i, $p(x_i) = 1$

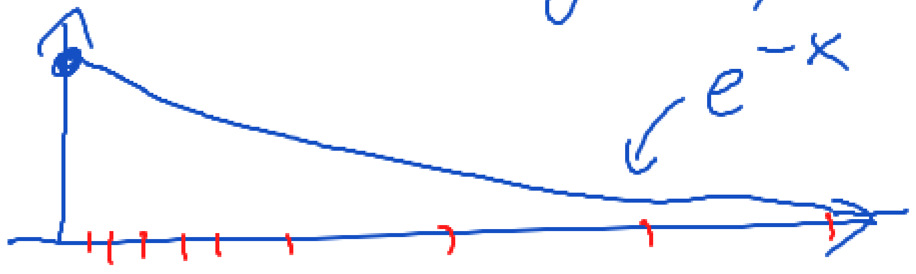
Method 2: $\overline{f}_N = \frac{1}{N} \sum_{i=1}^{N} e^{-\frac{x_i}{2}}$ w. RN x_i distr. acc. to $g(x_i) = e^{-x_i/2}$

$$I = \int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)}\, g(x)\,dx = \int_a^b \frac{e^{-x}}{e^{-x/2}}\, e^{-x/2}\,dx$$

$$= \int_a^b \underbrace{e^{-x/2}}_{\overline{f}_N}\ \underbrace{e^{-x/2}}_{RN\ x_i}\,dx$$



IS: Summary Importance Sampling: if $f(x)$ is small in large part of definition set, that region contributes little to the integral I — therefore we need less points x_i there to approximate I. We need x_i more in regions, where $f(x_i)$ is large (important)



M: Even more difficult cases can be solved by Metropolis algorithm. „Random Walk"

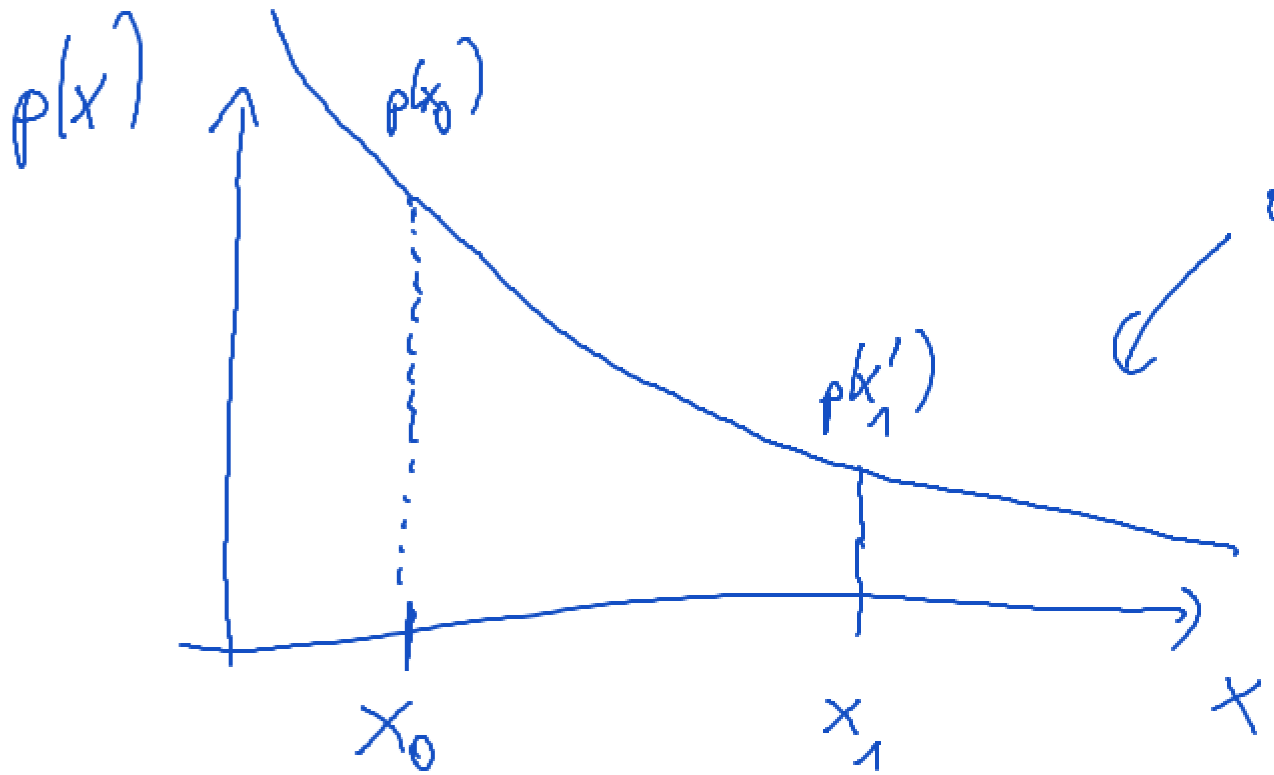
Special Form of Importance Sampling!

IS: $x_0, x_1, x_2, \ldots \; x_i \ldots$

M: $x_0', x_1' \xrightarrow{W} x_2', \ldots \; x_i' \xrightarrow{W} x_{i+1}'$

PDF $e^{-x_i/2}$

Transition Probability $W(x', x)$ is from $x \to x'$



$e^{-x/2}$

$$p(x_0) > p(x_1)$$

$$\underbrace{W(x_1, x_0)}_{x_0 \to x_1} < \underbrace{W(x_0, x_1)}_{x_1 \to x_0}$$