9.1. Monte Carlo Integration

$p(\vec{x})$ PDF for random vectors $\vec{x} \in \mathbb{R}^n$ $(V \subseteq$

(some average)

$\langle f \rangle_p$ expectation value of f over p

$$\langle f \rangle_p = \int_V f(\vec{x})\, p(\vec{x})\, d\vec{x} \;; \quad V = \int_V d\vec{x}$$

In case of equally distributed PDF:

$$p(\vec{x}) = \frac{1}{V} = \text{const.} \quad \int_V p(\vec{x})\, d\vec{x} = 1$$

In the following keep to 1D case:

$$\langle f \rangle_p = \int_a^b f(x)\, p(x)\, dx \quad \left[\text{if const. PDF } p(\vec{x}) = \frac{1}{b-a} \right] = \frac{1}{b-a} \int_a^b f(x)\, dx$$

Squared Expectation value (mean square) (second moment)

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

$\boxed{\text{r.m.s = root mean square} = \langle \ldots \rangle_p^{1/2}}$

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

[r].m.s.deviation

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

Variance of f over p:

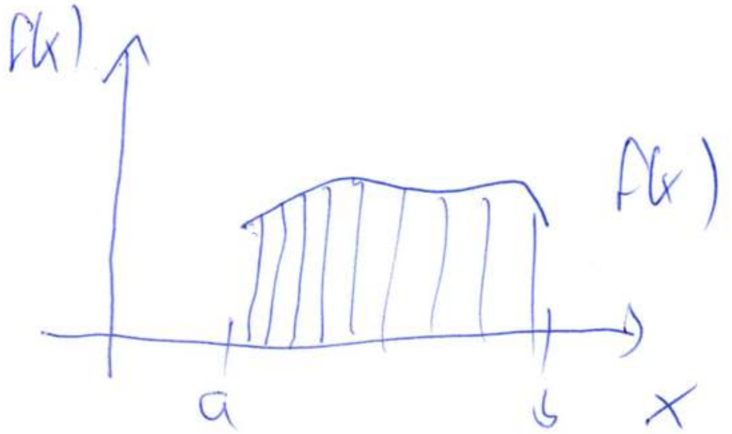
$$\sigma^2 = Var(f) = \int (f - \langle f \rangle_p)^2\, p(x)\, dx$$

Empirical approximation of exp. value by finite set of random numbers:

$$\overline{f_N} = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \qquad \overline{f_N^2} = \frac{1}{N}\sum_{i=1}^{N} f(x_i)^2$$

$\lim_{N\to\infty} \overline{f_N} = \langle f \rangle_p$ $\quad \lim_{N\to\infty} \overline{f_N^2} = \langle f^2 \rangle_p$

using x_i distributed according to $p(x)$



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

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

They are called empirical mean and second moment.

By law of large numbers (Central Limit theorem) many $\overline{f_N}$ samples have a Gaussian distribution around the expectation value $\langle f \rangle_p$ with variance

$$\langle f \rangle_p = \overline{f_N} \pm \sigma_N(f) \qquad \lim_{N\to\infty} \overline{f_N} = \langle f \rangle$$

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

Conclusion:

- Determine $\langle f \rangle_p = \int f(x) p(x) dx$ in this way error decreases with $N^{-1/2}$ only! MC worse than other num. integrators!
- But robust and easy to use, esp. in multi-dimensional case.

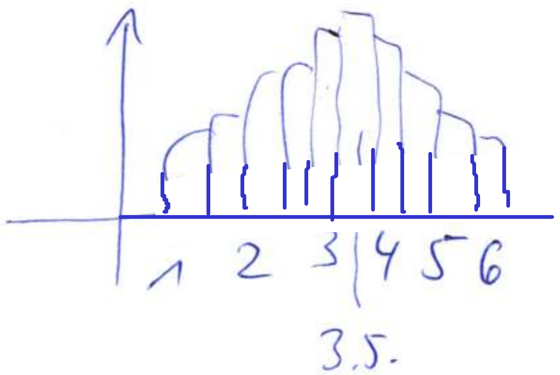
Simple Demonstration of Central Limit Theorem:

Rolling Dice: $\overline{f_N} = \frac{1}{N} \sum x_i$ $\quad 1 \leq x_i \leq 6$

One „Sweep": N times rolling dice

Expectation value for average: $\langle f \rangle = 3.5$

Many „Sweeps": Distribution of averages



Gaussian Distribution around $\langle f \rangle$

with $\sigma_N^2 \propto \frac{1}{N-1}$

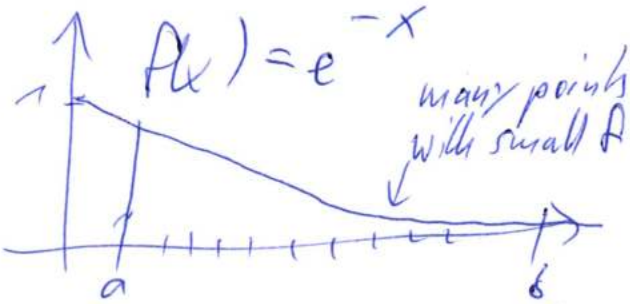
Importance Sampling

$$\langle f \rangle_p = \int_a^b f(x) p(x)\, dx \;; \quad \text{with } p(x) = \text{const.} = \frac{1}{b-a}$$

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

(*) With $\overline{f}_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$ we can approximate $\langle f \rangle_p = I/(b-a)$

But if $f(x)$ is small for large parts of definition set, equally distributed RV's are inefficient for sampling f



Choose $g(x)$ „near" $f(x)$:

$$I = \int_a^b \frac{f(x)}{g(x)} g(x)\, dx \;; \quad \text{choose RV's with PDF } g(x): 1 = \int_a^b g(x)\, dx$$

Then

(**) $\overline{f}_N = \frac{1}{N} \sum \frac{f(x_i)}{g(x_i)}$ approximates I with RN distr. as $g(x_i)$

Note: in (*) we approx. $\langle f \rangle_p = I/b-a$; in (**) I directly approx.!!

Example: Method 1: $\overline{f}_N = \frac{1}{N} \sum e^{-x_i}$ x_i equally distr.

Method 2: $\overline{f}_N = \frac{1}{N} \sum e^{-x_i/2}$ x_i with PDF $c \cdot e^{-x_i/2}$!
(get with transformation)! c by normalization cond.!

Example: $f(x) = e^{-x}$

Method 1: $\overline{f_N} = \frac{1}{N} \sum_{i=1}^{N} e^{-x_i}$ x_i w. $p(x_i) \equiv 1$

Method 2: $\overline{f_N} = \frac{1}{N} \sum_{i=1}^{N} e^{-\frac{x_i}{2}}$ x_i w. PDF $e^{-x_i/2}$

Metropolis Algorithm:

$\langle f \rangle_p = \int p(x) f(x) dx$

$f_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$ $x_i \leftrightarrow p(x_i)$

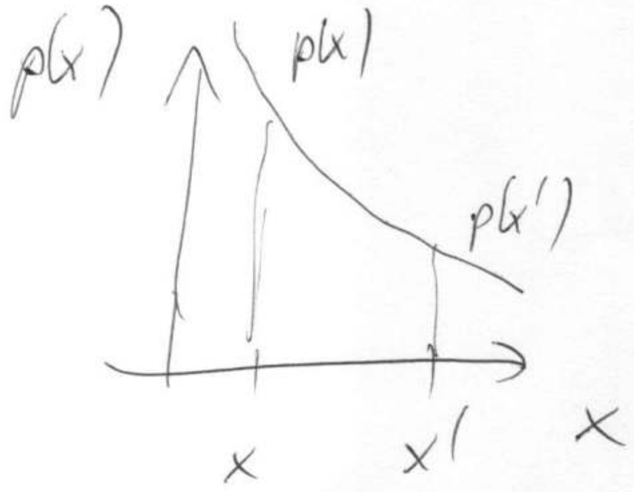
Realize $p(x_i)$ as equilibrium function of a Markoff* process

$x \to x'$ probability $W(x', x)$

* process without memory (no correlation with previous steps), stochastic, Master eq.

Realize eq. by detailed balance:

$$W(x,x')\,\rho(x') = W(x',x)\,\rho(x)$$



$\rho(x) > \rho(x')$

$W(x',x) < W(x,x')$

MRRTT algorithm:

$$W(x,x') = \gamma\,\Theta\,\min\left(1, \frac{\rho(x)}{\rho(x')}\right)$$

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$\Theta = \Theta(\delta - |x-x'|)$ limit , $\gamma = 1$

Start : RN x_i , $\rho(x_i) = x$

Step : RN x_{i+1} , $\rho(x_{i+1}) = x'$

If $\rho(x') > \rho(x)$: accept

If $\rho(x') < \rho(x)$: RN $\tilde{x}$; accept if $\tilde{x} < \frac{\rho(x')}{\rho(x)}$

- Do i steps for initialization
- Then N steps for measurement
  store x_i, $i=1,\dots N$

$$f_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

(This is one sweep)

- Do again N steps to get new measurement values

$$\langle f \rangle_p \cong \frac{1}{N_S} \sum_{\text{sweeps}} f_N$$