Repetition / Summary: We have approximated

- expectation values $\langle f \rangle_p = \int_a^b f(x)\, p(x)\, dx$
- integrals $I = \int_a^b f(x)\, dx$

If $p(x)$ eq. distributed $\Rightarrow p(x) = \frac{1}{b-a} \Rightarrow$

$$\langle f \rangle_p = \frac{1}{b-a} I \iff I = (b-a) \langle f \rangle_p$$

If $a=0, b=1$ : $b-a=1 \iff I = \langle f \rangle_p$

Methods used for approximation:

(1) $\bar{f}_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$ $\quad$ $x_i$ distr. acc. to $p(x_i) = \text{const.}$

$\langle f \rangle_p = J/(b-a)$

(2) $\bar{f}_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$ $\quad$ $x_i$ distr. acc. to $p(x_i)$ not const.

$\langle f \rangle_p$

(3) $\bar{f}_N = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{g(x_i)}$ $\quad$ with $x_i$ distr. acc. to $g(x_i)$

Importance Sampling

approximates: $J = \int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)}\, g(x)\,dx$

$= \left\langle \frac{f(x)}{g(x)} \right\rangle_g$

Metropolis Algorithm:

yet another method to generate a non-trivial $p(x_i)$, PDF

($p(x)=1$ LCG's; transformation method, rejection, Box-Muller)

$$\langle f \rangle_p = \int f(x)\, p(x)\, dx \;; \quad \overline{f}_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \qquad x_i \text{ distr. acc. to } p(x_i)$$

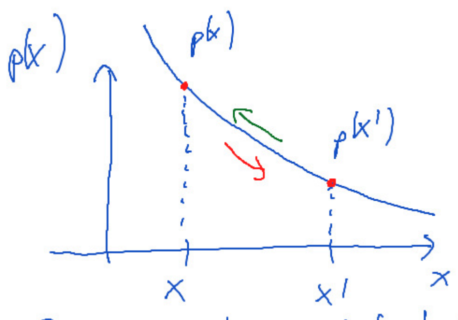
(in prep. for Ising-Model: we need some method to realize a PDF $p(x_i)$ which is extremely small in large parts of definition set!)

(Even importance sampling will fail for Ising model!)

Realize $p(x_i)$ as equilibrium function of a Markoff* process (random walk, random process, follows some rules)

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

* process without memory (no correlation with previous steps; stochastic, not deterministic; reach all parts of def. set; Master eq.




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

Realize by detailed balance:

$$W(x,x')\,p(x') = W(x',x)\,p(x) \qquad (1)$$

MRRTT = Metropolis, Rosenbluth, Teller; simplest definition to get Markoff:

$$W(x,x') = \gamma\,\tilde\Theta \min\left(1,\ p(x)/p(x')\right) \qquad (2)$$
$$W(x',x) = \gamma\,\tilde\Theta \min\left(1,\ p(x')/p(x)\right)$$

$p(x) > p(x')$

$x' \to x \Rightarrow W = 1$

$x \to x' \Rightarrow W = \frac{p(x')}{p(x)} < 1$

$$\tilde\Theta = \Theta(\delta - |x-x'|);\ \Theta = 0 \text{ if } |x-x'| > \delta;\ \gamma = 1$$

Start of the Metropolis process:

RN $x_0$ , $x_1$ from. eq. distr. RN from full def. set!

$\Rightarrow p(x_0), p(x_1)$ ; $x_0 = x$ ; $x_1 = x'$

(i) If $p(x') > p(x)$: accept!

(ii) If $p(x') < p(x)$: RN $\tilde{x}$ eq. distr. $[0,1]$ ; accept if $\tilde{x} < \frac{p(x')}{p(x)}$

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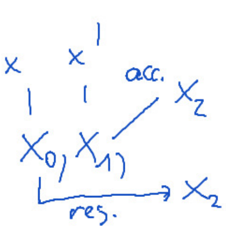
Example: $p(x') = \frac{1}{2} p(x)$ ; $p(x') < p(x)$ case (ii)

RN $\tilde{x}$, eq. distr. $0 \leq \tilde{x} \leq 1$ $\quad \tilde{x} \gtrless \frac{p(x')}{p(x)} = 0.5$ $\longleftrightarrow W(x';x)$




Probability that $x'$ is accepted is 0.5 (50%)

$W(x',x) = 0.5$

Metropolis algorithm gives sequence of $x_i$, follow $p(x_i)$

$x_0, x_1, \ldots, x_i, x_{i+1}, \ldots$

- Do $i$ steps for initialization! „thermalization" equilibrate
- Then $N$ steps $\ldots x_i, x_{i+1}, \ldots, x_{i+N}, \ldots$

$$\bar{f}_{N,j} = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

This is called one sweep! Sweep number $j$

- Do again $N$ steps to get next sweep; in total $N_s$ sweeps

$$\langle f \rangle_p \sim \frac{1}{N_s}\sum_{j=1}^{N_s} \bar{f}_{N,j}$$



Distr. of $\bar{f}_{N,j}$