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

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

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

Metropolis Algorithm:

$$\langle f \rangle_p = \int_x p(x) f(x) \, dx$$

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

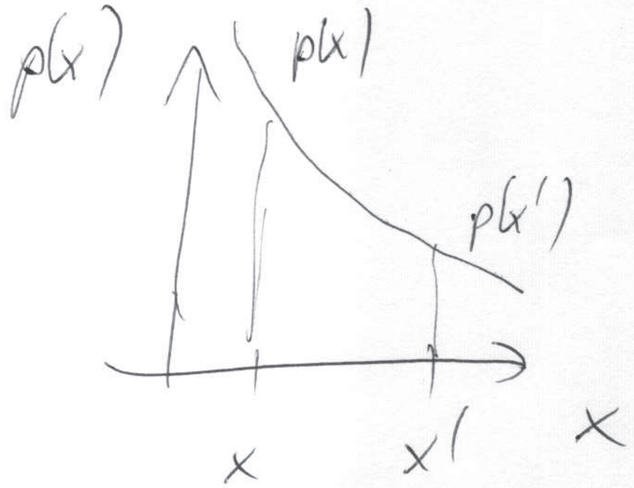
Realize $p(x_i)$ as equilibrium function of a Markoff* process

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

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

Realize ~~eeq.~~ 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:

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

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

$\Theta = \Theta(\delta - |x-x'|)$ 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 $x_i, i = 1, \ldots N$

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

(This is one sweep)

- Do again N steps to get new measurement values

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