METROPOLIS ALGORITHM: AN EXAMPLE

Let $\pi(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}$ on $\mathbb{R}$

STATE SPACE : continuous variable in $\mathbb{R}$

DYNAMICS : At time t the system is in x: $x_t = x$
We must define x_{t+1}, the position at time $t+1$.

We FIX p (parameter that defines $P^{(0)}$) [IT CAN BE OPTIMIZED]

STEP 1 (PROPOSAL) : We choose y uniformly in the interval $[x-p, x+p]$

STEP 2 (ACCEPTANCE) : We accept y with probability A_{xy}

We now verify that $P^{(0)}_{xy}$ is SYMMETRIC

Choose two points x and y and ϵ small (infinitesimal)

If $|x-y| > p \Rightarrow P^{(0)}_{xy} = P^{(0)}_{yx} = 0$

Correction: replace epsilon with epsilon/(2 p)

If $|x-y| < p \Rightarrow \begin{cases} \text{Prob}(x \to [y, y+\epsilon]) = \epsilon \\ \text{Prob}(y \to [x, x+\epsilon]) = \epsilon \end{cases}$ EQUAL

For a symmetric $P^{(0)}_{xy}$ we have

$$R_{xy} = \frac{\pi_y P^{(0)}_{yx}}{\pi_x P^{(0)}_{xy}} = \frac{\pi_y}{\pi_x} = e^{x^2-y^2}$$

It follows

$$A_{xy} = \min\left(1, e^{x^2-y^2}\right)$$

IMPLEMENTATION OF ONE ITERATION

SET $X = X_{i-1}$

$y = X + 2p\,(\mathrm{RAN}(\ ) - 0.5)$ (PROPOSAL)

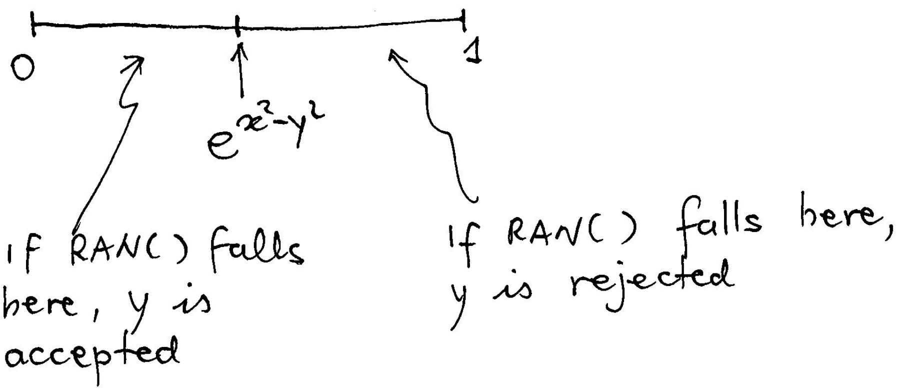
$\text{if } (y < x) \quad x_1 = y$

$$\text{else} \begin{cases} \text{if } \left(e^{x^2-y^2} < \mathrm{RAN}(\ )\right) & x_1 = x \quad \text{(REJECTED)} \\ \text{else} & x_1 = y \quad \text{(ACCEPTED)} \end{cases}$$

COMMENTS

- $2p(\mathrm{RAN}(\ ) - 0.5)$ gives a random number uniformely distributed in $[-p, p]$
- if $y \leq x$, $e^{x^2-y^2} > 1$ so that $A_{xy} = 1$ the move is accepted
- if $y > x$, $e^{x-y^2} < 1$ so that $A_{xy} = e^{x^2-y^2}$ In this case we should accept y with probability $e^{x^2-y^2}$

  The strategy is the following



ANOTHER ALGORITHM (useful for simulated tempering / parallel tempering)

STATE SPACE: 5 discrete points

PROBABILITY: $\pi_x = \{ \pi_1, \pi_2, \pi_3, \pi_4, \pi_5 \}$

DYNAMICS:

STEP 1: (proposal)

$$\begin{cases} \text{if } x = 2,3,4 \text{ we propose} \begin{cases} y = x+1 & \text{prob. } 1/2 \\ y = x-1 & \text{prob } 1/2 \end{cases} \\ \text{if } x = 1 \text{ we propose } y = 2 \text{ with prob } 1 \\ \text{if } x = 5 \text{ we propose } y = 4 \text{ with prob } 1 \end{cases}$$

STEP 2: (acceptance) we accept y with prob A_{xy}.

In this case $P^{(0)}_{xy}$ is not symmetric

The proposal can be implemented as follows

$[x = x_{t-1}]$

if $(x=1)$ $y = 2$

$$R = \frac{P^{(0)}_{21}\,\pi_2}{P^{(0)}_{12}\,\pi_1} = \frac{\pi_2}{2\pi_1}$$

if $(x=2)$ if (RAN( ) < 0.5) $y = 1$

$$R = \frac{P^{(0)}_{12}\,\pi_1}{P^{(0)}_{21}\,\pi_2} = \frac{2\pi_1}{\pi_2}$$

else $y = 3$

$$R = \frac{P^{(0)}_{32}\,\pi_3}{P^{(0)}_{23}\,\pi_2} = \frac{\pi_3}{\pi_2}$$

if $(x > 2$ && $x < 4)$ if (RAN( ) < 0.5) $y = x + 1$
else $y = x - 1$

$$R = \frac{\pi_y}{\pi_x}$$

if $(x = 4)$ if (RAN( ) < 0.5) $y = 3$

$$R = \frac{P^{(0)}_{34}\,\pi_3}{P^{(0)}_{43}\,\pi_4} = \frac{\pi_3}{\pi_4}$$

else $y = 5$

$$R = \frac{P^{(0)}_{54}\,\pi_5}{P^{(0)}_{45}\,\pi_4} = \frac{2\pi_5}{\pi_4}$$

if $(x = 5)$ $y = 4$

$$R = \frac{P^{(0)}_{45}\,\pi_4}{P^{(0)}_{54}\,\pi_5} = \frac{\pi_4}{2\pi_5}$$

The move is accepted with probability min $(1, R)$ and can be implemented as follows

if $(R \geq 1)$ $x_i = y$
else if (RAN( ) < R) $x_i = y$
else $x_i = x_{i-1}$ (rejection)

EXERCISE:

We can also define a symmetric proposal:

if $x = 2,3,4$ we propose $\begin{cases} y = x+1 & \text{prob } 1/2 \\ y = x-1 & \text{prob } 1/2 \end{cases}$

if $x = 1$ we propose $\begin{cases} y = 2 & \text{prob } 1/2 \\ y = 1 & \text{prob } 1/2 \end{cases}$

if $x = 5$ we propose $\begin{cases} y = 5 & \text{prob } 1/2 \\ y = 4 & \text{prob } 1/2 \end{cases}$

As an exercise show that $p^{(0)}_{xy} = p^{(0)}_{yx}$ for all (x,y).

QUESTION: is this dynamics more efficient or less efficient than the first one?

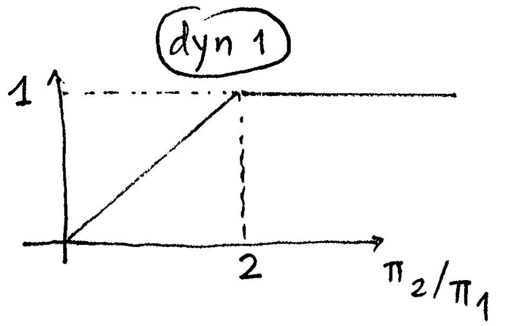
There is a difference only at the boundaries
Let's compute P_{12} for the two dynamics

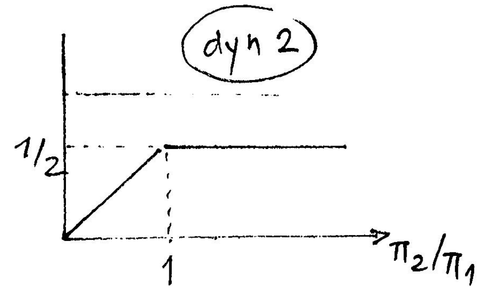
dynamic 1: $P_{12} = P^{(0)}_{12} A_{12} = 1 \times \min\left(1, \frac{\pi_2}{2\pi_1}\right)$

$$= \min\left(1, \frac{\pi_2}{2\pi_1}\right)$$

dynamic 2: $P_{12} = P^{(0)}_{12} A_{12} =$

$$= \frac{1}{2} \min\left(1, \frac{\pi_2}{\pi_1}\right)$$





DYN 1 is MORE efficient