The Metropolis algorithm

The Metropolis algorithm is a general purpose algorithm, which can be applied to essentially any problem.

Let us recall our problem: given a probability distribution $\pi$ on a state space $S$, we wish to determine a transition matrix $P$ which has $\pi$ as equilibrium distribution.

The Metropolis algorithm is made of two different steps.

(i) **Step 1.** The system is currently (time $i$) in state $x_i = x$. We propose a new configuration $y \neq x$ of the system with a proposal transition matrix $P^{(0)}$. The proposal matrix is arbitrary (it has no relation with the probability $\pi_x$) and is chosen by the programmer.

(ii) **Step 2.** Now we establish if the proposed new configuration $y$ should be accepted or rejected. We accept it with probability $A_{xy}$. If the configuration $y$ is accepted, we set $x_{i+1} = y$; otherwise $x_{i+1} = x_i$. The acceptance matrix depends on the proposal matrix and on the probability distribution $\pi_x$. The matrix $A_{xy}$ is a probability and therefore satisfies $0 \leq A_{xy} \leq 1$. 
We now compute the Metropolis transition matrix $P_{xy}$ (the probability of going from $x$ to $y$).

For $y \neq x$, the probability of going from $x$ to $y$ is the product of the probability of proposing $y$ times the probability of accepting the proposed move:

$$P_{xy} = P_{xy}^{(0)} A_{xy} \quad x \neq y$$

The probability of remaining in $x$ is obtained by using the conservation of probability

$$P_{xx} = 1 - \sum_{y \neq x} P_{xy} = P_{xx}^{(0)} + \sum_{y \neq x} P_{xy}^{(0)} (1 - A_{xy}).$$

The two terms represent the probability of proposing no change ($P_{xx}^{(0)}$) and the sum of the probabilities that the proposed moves are not accepted. We used

$$1 = \sum_{y} P_{xy}^{(0)} = P_{xx}^{(0)} + \sum_{y \neq x} P_{xy}^{(0)}.$$
To have a valid we require that $P$ is an ergodic Markov process and that the detailed balance condition is satisfied.

Necessary (but not sufficient) condition for $P$ to be ergodic is that $P^{(0)}$ is ergodic. The ergodicity of $P$ should be verified explicitly (it is usually trivially satisfied if the system is characterized by countinuous variables; more subtle is checking ergodicity for systems with discrete variables).

Now we require $P$ to satisfy the detailed-balance condition $\pi_x P_{xy} = \pi_y P_{yx}$ for any pair of states $x, y$, The condition becomes

$$\pi_x P_{xy}^{(0)} A_{xy} = \pi_y P_{yx}^{(0)} A_{yx}$$

i) If $x, y$ are such that $P_{xy}^{(0)} = P_{yx}^{(0)} = 0$ (we never propose to go from $x$ to $y$ ore vice versa) the condition is satisfied.

ii) If $x, y$ are such that $P_{xy}^{(0)} = 0$ and $P_{yx}^{(0)} > 0$, we set $A_{yx} = 0$. If the system never goes from $x$ to $y$, it should not go from $y$ to $x$. Analogously, if $x, y$ are such that $P_{xy}^{(0)} > 0$ and $P_{yx}^{(0)} = 0$, we set $A_{xy} = 0$.

iii) If $x, y$ are such that $P_{xy}^{(0)} > 0$ and $P_{yx}^{(0)} > 0$. The detailed-balance condition requires that

$$\frac{A_{xy}}{A_{yx}} = \frac{\pi_y P_{yx}^{(0)}}{\pi_x P_{xy}^{(0)}}$$
The right-hand side is known and we call it $R_{xy}$:

$$R_{xy} = \frac{\pi_y P_{yx}^{(0)}}{\pi_x P_{xy}^{(0)}}$$

which satisfies

$$R_{xy} = \frac{1}{R_{yx}}.$$

Now, the problem is: determine the acceptance matrix $A_{xy}$ so that it satisfies the equation

$$\frac{A_{xy}}{A_{yx}} = R_{xy}$$

The Metropolis choice consists in taking

$$A_{xy} = \min(1, R_{xy})$$
Let us verify that this is a solution of the equation written above. Two cases: i) $R_{xy} > 1$; ii) $R_{xy} < 1$.

**Case i)**: $R_{xy} > 1$, so that $R_{yx} = 1/R_{xy} < 1$. Therefore, we have

$$A_{xy} = 1, \quad A_{yx} = R_{yx} \rightarrow \frac{A_{xy}}{A_{yx}} = \frac{1}{R_{yx}} = R_{xy}$$

**Case ii)**: $R_{xy} < 1$, so that $R_{yx} = 1/R_{xy} > 1$. Therefore, we have

$$A_{xy} = R_{xy}, \quad A_{yx} = 1 \rightarrow \frac{A_{xy}}{A_{yx}} = R_{xy}$$
The Metropolis choice is the optimal one. It gives the largest acceptance probability.

\[ A_{xy} = R_{xy}A_{yx} \leq R_{xy} \]

because \( A_{yx} \leq 1 \). Moreover \( A_{xy} \leq 1 \). It follows the inequality

\[ A_{xy} \leq \min(1, R_{xy}) \]