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 π on a state space S, we wish to determine a transition matrix P which has π 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 π_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 π_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 the product of the probability of proposing y times the probability of accepting the proposed move:

$$P_{xy} = P^{(0)}_{xy} A_{xy} \qquad\qquad x \neq y$$

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

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

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

$$1 = \sum_{y} P^{(0)}_{xy} = P^{(0)}_{xx} + \sum_{y \neq x} P^{(0)}_{xy}\,.$$

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}:

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

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

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

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

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

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

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