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Metropolis Algorithm

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Definition

The Metropolis algorithm is a *Monte Carlo method* advanced by Metropolis et al. (1953) to generate samples from a prespecified target probability distribution. Originally, it was applied to investigate the statistical mechanics of fluids. By now, this method and its extensions are used for a wide range of problems in scientific computing (see, e.g., Liu (2004)). The basic idea is to simulate a Markov chain so that its stationary distribution is the target distribution.

Let $\mathbb{X}$ be a discrete state space (finite or countable) on which the target probability distribution $\pi = (\pi_x)_{x\in\mathbb{X}}$ is defined. It is assumed that $\pi_x > 0,\ x \in \mathbb{X}$. Suppose that Q is a symmetric transition probability matrix, that is $Q = \left(q_{xy}\right)_{x,y\in\mathbb{X}}$ with $q_{xy} \geq 0,\quad q_{xy} = q_{yx},\quad \sum_{y\in\mathbb{X}} q_{xy} = 1, x, y \in \mathbb{X}.$ The following algorithm generates values (*realizations*) $x_0, x_1, \ldots$ of a Markov chain $X_0, X_1, \ldots$. Given the current state $X_t = x$ the next state X_{t+1} is determined by the following:

1. Choose a proposal state $y \in \mathbb{X}$ randomly according to the probability vector $Q_x := \left(q_{xy}\right)_{y\in\mathbb{X}}$.
2. Calculate the acceptance probability $\alpha = \min\{1, \pi_y/\pi_x\}$.
3. Accept the proposal by setting $X_{t+1} := y$ with probability α, or ignore the proposal by setting $X_{t+1} := x$ with probability $1 - \alpha$.

The stationary distribution of the Markov chain $X_0, X_1, \ldots$ constructed in this way is automatically π (Madras 2002). After some relaxation time, the chain generates samples from the target distribution, independent of the starting value. This allows to compute approximations of the mean value or higher moments of the distribution.

The Metropolis algorithm is particularly powerful, when the state space on which the probability distribution is defined consists of spatial configurations of particles (individuals, cells, etc.) that underlie a certain interdependence structure. The moments of the system then correspond to macroscopic variables that are often only numerically computable. In these applications, the space is discretized to ensure the discreteness of the state space. Then, a configuration η (of cells, particles, ...) can be understood as an element of $\mathbf{X} := W^S$, where $S \subset \mathbb{Z}^d$ is a regular lattice. The finite set W consists of all considered cell types or states (orientation, mass, cell cycle phase, sensitivity, etc.). The interpretation is that at each lattice node, there can be at most one cell with a certain cell type from W. Each cell's state shall depend on the states of its neighboring cells. Then, the overall interdependence structure can be described by a *Hamilton function* H: $\mathbf{X} \to \mathbb{R}$, which leads, for instance, to the target probability distribution

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$$\pi(\eta) = Z^{-1} \exp\{-H(\eta)\}, \qquad \eta \in \mathbb{X}$$

where Z is a normalizing constant. In this situation, a variant of the Metropolis algorithm, the so-called Glauber dynamics, is given by the following:

(0) Start with configuration η.

(1) Pick a target site $x \in S$ at random with uniform distribution on S.

(2) Pick a state w from W randomly with uniform distribution.

(3) Calculate the energetic difference $\Delta \mathrm{H}_x^w := H(\eta_x^w) - H(\eta)$ of a transition $\eta \to \eta_x^w$, where $\eta_x^w(z) := w$ if $z = x$ and $\eta_x^2(z) := \eta(z)$ otherwise.

(4) Accept the transition by setting $\eta := \eta_x^w$ with probability $p(\Delta \mathrm{H}_x^w)$, or ignore the transition with probability $1 - p(\Delta \mathrm{H}_x^2)$, where

$$p(\Delta \mathrm{H}_x^w) = \begin{cases} 1 & \text{if} \Delta \mathrm{H}_x^w < 0 \\ e^{-\Delta \mathrm{H}_x^w} & \text{otherwise} \end{cases}$$

(5) Go to (1) or end the algorithm.

References

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Madras NN (2002) Lectures on Monte Carlo methods. Fields Institute monographs, American Mathematical Society, Providence

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