Notes on Monte Carlo

A Preprint

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Abstract

Notes on monte carlo.

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1 Introduction

Importance sampling

Using monte carlo to reproduce a Boltzmann distribution

2 Importance Sampling

A stochastic process that obeys the conditions of a Markov process will reproduce a Boltzmann distribution.

A discrete-time Markov chain is the simplest sort of stochastic process.

2.1 Markov Chains

A Markov chain is a process in which the probability $P(\nu \to \mu)$ of making a transition from state ν to state μ depends only on those two states.

$P(\nu \to \mu)$ must be constant over time. And $\Sigma_\mu P(\nu \to \mu) = 1$. Also, there can be a non-zero probability of remaining in the same state, that is $P(\mu \to \mu) \neq 0$.

Right now, with these constraints, you should be thinking of a random walk! In order to reproduce a Boltzmann distribution we need two more requirements.

The first is that it must be possible to reach any state from any other state though a finite number of transitions. This is the condition of **ergodicity**. Mathematically, this corresponds to having non-zero boltazmann factors at all times.

The second condition normally goes by the name of **detailed balance**. Simple "balance" tells us that after the system has come to equilibrium the rate of transition into any given state equals the rate of transition out of that state

$$\Sigma_\mu p_\nu P(\nu \to \mu) = \Sigma_\mu p_\mu P(\mu \to \nu) \tag{1}$$

Here, p_μ corresponds to the probability of the system of being in state μ. And $P(\nu \to \mu)$ corresponds to the transition probability of going from state ν to state μ.

This condition, however, does not rule out a state of dynamic equilibrium. Say something about dynamic equilibrium [1].

In order to reproduce a Boltzmann distribution we need to guarantee a state of static equilibrium. This is where detailed balance comes in. The idea of detailed balance builds on top of the normal balance condition of (1). Detailed balance requires that the rate at which the system transitions into a state μ from a state ν must be equal to the rate at which it transitions from μ to ν

$$p_\nu P(\nu \to \mu) = p_\mu P(\mu \to \nu) \tag{2}$$

Equation (2) can be used to set the Boltzmann factor

$$\frac{P(\nu \to \mu)}{P(\mu \to \nu)} = \frac{p_\mu}{p_\nu} = e^{-\beta(E_\mu - E_\nu)} \tag{3}$$

2.1.1 Computational Details

In practice we will want to break up the transition probabilities into a product of generation and acceptance probabilities such as

$$\frac{P(\nu \to \mu)}{P(\mu \to \nu)} = \frac{g(\nu \to \mu)}{g(\mu \to \nu)} \frac{A(\nu \to \mu)}{A(\mu \to \nu)} \tag{4}$$

Where $g(\nu \to \mu)$ is the probability of producing a state μ from a state ν and $A(\nu \to \mu)$ the prbability of acception the state μ that has been generated from a state ν.

In the perfect case, the acceptance probabilities would be as close to unity as possible - whatever state that is generated is accepted and we are sampling the most important details of our system.

3 Ising Model

Now that we got some theory out of the way, it is time to explore some Markov chain Monte Carlo algorithms. We will begin by intrducing the Ising model and to discuss how to simulate it in a lattice using the Metropolis and the Wolff cluster algorithms.

3.1 Model description

The Ising model is intended to describe ferromagnetic meterials. Its formulation is a magnet being composed of "spins", each spin corresponding to a point in a lattice. A spin can take a value of either +1 or -1 (a magnetic dipole pointing up or down). Its Hamiltonian being

$$H = -\sum_{<ij>} J_{ij} s_i s_j - \sum_i B_i s_i \tag{5}$$

$\sum_{<ij>}$ indicates a sum over all pairs of neighboring spins; J_{ij} the strength of the interaction between neighboring spins; B the strength of the external magnetic field at position i; and s_i is the spin at site i, $s_i \in \{+1, -1\}$.

3.2 Figures

See Figure 1. Here is how you add footnotes. [1]

References

[1] Lee J. Silverberg and Lionel M. Raff. Are the Concepts of Dynamic Equilibrium and the Thermodynamic Criteria for Spontaneity, Nonspontaneity, and Equilibrium Compatible? In *J. Chem. Educ. 2015, 92, 4, 655-659*. Publication Date: January 23, 2015. https://doi.org/10.1021/ed500660j

[2] George Kour and Raid Saabne. Fast classification of handwritten on-line arabic characters. In *Soft Computing and Pattern Recognition (SoCPaR), 2014 6th International Conference of*, pages 312–318. IEEE, 2014.

[3] Guy Hadash, Einat Kermany, Boaz Carmeli, Ofer Lavi, George Kour, and Alon Jacovi. Estimate and replace: A novel approach to integrating deep neural networks with existing applications. *arXiv preprint arXiv:1804.09028*, 2018.

[1] Sample of the first footnote.

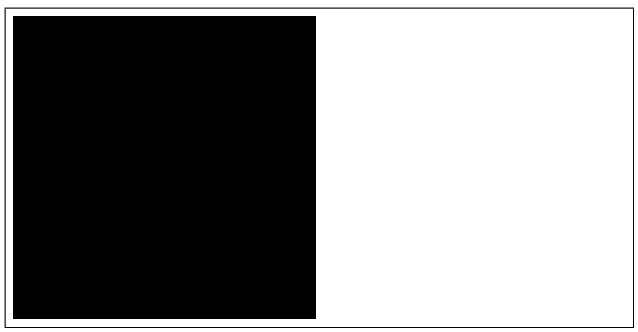

Figure 1: Sample figure caption.