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# Metropolis-Hastings Algorithm

**8. Task for Model Analysis I, 2023/24**

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# Contents



# 1 Introduction

We're continuing our exploration into random numbers and their applications. Previously we had a look at Monte Carlo sampling. Today we're going to delve into the Metropolis-Hastings algorithm, which can be thought of as Monte Carlo sampling with a few extra steps. Since our end goal is to simulate the relaxation of a lattice of spins in a magnetic field, we'll take the Ising model as our physical context.

We know from statistical physics that the 2D Ising model relaxes to a state of minimum energy. We can simulate this relaxation by flipping spins at random and accepting or rejecting the new state based on the change in energy. We can have a negative change of energy which we can call a *good move* or a positive change of energy which we can call a *bad move*. The added twist with this algorithm is that while we always accept the new state if we make a good move, we also sometimes accept a new state after a bad move. This is the key to the Metropolis-Hastings algorithm. Given our system the probability of accepting a bad move is given by the Boltzmann factor and the temperature of the system:

$$P_{\text{bad accept}} = \exp\left(-\frac{\Delta E}{kT}\right) , \tag{1}$$

where $\Delta E$ is the change in energy, $k$ is the Boltzmann constant and $T$ is the temperature. Why exactly this works is a bit more involved and probably out of the scope of this report however a dedicated reader can find more information in this well written blog post by Gregory Gundersen of Princeton University [1]. We can define multiple different exit conditions for the algorithm, such as a fixed number of iterations, a fixed number of accepted moves or an $\varepsilon$ tolerance for $\Delta E$.

# 2 Task at Hand

## 2.1 Molecular Chain

The instructions given demand that we first explore the Metropolis-Hastings algorithm on a simple molecular chain. The molecular chain is made up of 17 molecules that can go from a state of 0 to a depth of $-18$. The deeper a molecule is the lower its potential energy. But we also have a positive energy contribution if neighboring bonds are very stretched. The final result is determining the equilibrium energy as a function of the temperature.

## 2.2 Ising Model

As mentioned in the intro our main goal is to simulate the relaxation of a lattice of spins in a magnetic field. We can describe a ferromagnetic material with the following Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,\, j \rangle} s_i s_j - H \sum_i s_i \, , \tag{2}$$

where $s_i$ is the spin of the $i$-th site, $H$ is the external magnetic field and $J$ is the coupling constant, which is positive for ferromagnetic materials and negative for antiferromagnetic materials. In the absence of a magnetic field the critical temperature for the transition from a paramagnetic to a ferromagnetic state is given by the Onsager solution approximately as:

$$T_c \approx 2.269185 \, \frac{J}{k_B} \, . \tag{3}$$

The instructions demand that we determine the average energy $\langle E \rangle$ and eigen-magnetization $\langle S \rangle$ as functions of temperature. The magnetization of the system is defined as:

$$S = \frac{1}{N} \sum_i s_i \, , \tag{4}$$

where $N$ is the number of spins. We can also have a look at spin susceptibility $\chi$ and heat capacity $c$ at different external magnetic field strengths. Spin susceptibility is defined as:

$$\chi = \frac{\langle S^2 \rangle - \langle S \rangle^2}{N k_B T} \, , \tag{5}$$

and heat capacity is defined as:

$$c = \frac{\langle E^2 \rangle - \langle E \rangle^2}{N k_B T^2} \, . \tag{6}$$

# 3 Solution Overview

# 4 Results

# 5 Conclusion and Comments

# References

[1] Gregory Gundersen. Why Metropolis-Hastings Works. https://gregorygundersen.com/blog/2019/11/02/metropolis-hastings/#bishop2006pattern, Nov 2019. [Accessed 24-07-2024].