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Metropolis-Hastings Algorithm

8. Task for Model Analysis I, 2023/24

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Contents

1	Introduction	1
2	Task at Hand	1
2.1	Molecular Chain	1
2.2	Ising Model	2
3	Solution Overview	2
3.1	Molecular Chain	2
3.2	Ising Model	2
4	Results	3
5	Conclusion and Comments	3

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:

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

where ΔE 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 ε tolerance for ΔE . Really that is all there is to this method from a theory standpoint.

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:

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

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:

$$T_c \approx 2.269185 \frac{J}{k_B}. \quad (3)$$

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:

$$S = \frac{1}{N} \sum_i s_i, \quad (4)$$

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

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

and heat capacity is defined as:

$$c = \frac{\langle E^2 \rangle - \langle E \rangle^2}{N k_B T^2}. \quad (6)$$

3 Solution Overview

This report marks a change in the way I approach these tasks for Model Analysis I. Up until now I've given heavy focus on the quality, optimization and performance of my code and have neglected the actual purpose of the subject, which is the analysis of physical models. The idea was that more advanced code or methods would allow me to do better analysis. However, the overhead of time needed to implement these methods was not worth the benefit. I don't think I've ever managed to show the results of my code since I've always been too focused on the code itself. It's time to change that. As much as it pains me I will try to employ a *good-enough* approach (aka. the *KISS* principle) and focus on the analysis of the models. I will still try to write clean and efficient code but I will not spend too much time on it, especially on paralelization and optimization. From a utilitarian perspective it's better to have a working solution that is not optimal than to have an optimal solution that took too long to implement.

3.1 Molecular Chain

I started writing the code for the molecular chain quite a long time ago before I burnt out. I threw all that old code away and started anew. As has become a bit of a habit I created a 1D Metropolis-Hastings solver class `Metropolis1` which I can then also reuse for the Ising model with minimal adaptations. The advantage of a class-based approach is that I can more easily do parameter sweeps as I can just create a new instance of the class with different parameters. Since I wanted to get decent statistics for the molecular chain I had quite strict exit conditions and also many repeat runs for each temperature. This produced quite a massive amount of data which I conveniently stored in a `HDF5` file. I ♥ `HDF5`.

3.2 Ising Model

After (re)writing the code for the molecular chain I adapted it for the Ising model, creating a solver class `Metropolis2`. I had a few problems with the scale of energy and temperature but I think I managed to solve those in the end and the results seem to be reasonable. Data was also stored in a `HDF5` file, due to the sheer volume as I wanted a decent sample size for my statistics. The main challenge was the code

being relatively slow per lattice and I wanted to simulate long times. As much as I promised not to focus on optimization I did to single-computer parallelization by utilizing the `ProcessPoolExecutor` from the `concurrent.futures` module of Python. As stated above, a class-based approach allowed me to easily spawn multiple instances of the solver class with different parameters on different processes which greatly sped up the gathering of data. I think this style of parallelization is reasonable as it takes very little time to implement and yields significant speedups. Here is a brief overview of how `ProcessPoolExecutor` is used:

```

1 import ...
2
3 class Worker:
4     def __init__(self,
5                 temperature: float,
6                 run: int,
7                 ):
8         self.T = temperature
9         self.run = run
10
11     def process(self):
12         dim = (50, 50)
13         m = Metropolis2(dim, self.T)
14         # Set parameters for the simulation
15         s_init, s_final, en = m.run()
16
17         return self.run, s_init, s_final, en, m.temperatures
18
19 # Create function that'll get the workers to work
20 def worker_task(params):
21     worker = Worker(*params)
22     return worker.process()
23
24 # Run process pool and save on thread execution
25 with concurrent.futures.ProcessPoolExecutor(max_workers=16) as executor:
26     futures = [executor.submit(worker_task, params) for params in param_list]
27
28     # Step 4: Collect the results
29     for future in concurrent.futures.as_completed(futures):
30         run, s_init, s_final, en, temps = future.result()
31         # Save data etc.

```

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].