Assignment 6: MCMC Simulation and Review Problems

Preface: In this assignment, you will use computational software to implement the Markov Chain Monte Carlo (MCMC) simulation algorithm we simulated ourselves in class.

1. **MCMC of Spins in a Magnetic Field**
   In this problem, we simulate spin system depicted in Fig. 1.

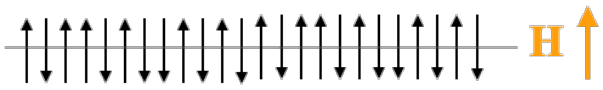

Figure 1: Particular microstate of the system we are simulating.

Using the partition function, we can show that for a collection of N spins each of which has magnetic dipole μ and subject to magnetic field H, the average spin is given by

$$\langle s \rangle = \tanh\left(\frac{\mu H}{k_B T}\right), \tag{1}$$

where $\tanh(x) = (e^x - e^{-x})/(e^x + e^{-x})$. We will use a simulation to compare the theoretical result Eq.(1) to one obtains from computation.

We will be using *Mathematica* to complete this problem, so we need to establish some code preliminaries.

(i) Log in to your account in one of MIT's Athena Clusters, and go to the MITES 2018 –Physics III course website.

(ii) Download the code `spin_model_simulation.nb` from the course webpage and open it in *Mathematica*.

(iii) Select a block of code and run it by pressing `Shift+Enter`.

Now we begin the problem

(a) Run each line of the "Function Definitions" section of the code to determine what the associated function does

(b) **Low Temperature Simulation**

Fill in all the "..." in the code. In particular define/fill in the following:

- Parameter definition $\mu = 1.0$, $H = 1.0$, $k_B T = 0.1$
- There are $N_{\text{spins}} = 1000$ in the system
- There are $N_{\text{steps}} = 10,000$
- An initial spin configuration with N_{spins} all of which have value -1;

- Energy of microstate is given by

$$E(\{s_i\}) = -\mu H \sum_{i=1}^{N} s_i \tag{2}$$

- The ratio between Boltzmann factors for final and initial spin configurations

$$\exp\left[-\frac{1}{k_B T}\left(E(\{s_i\}_{\text{final}}) - E(\{s_i\}_{\text{initial}})\right)\right] \tag{3}$$

- The theoretical value of $\langle s \rangle$ obtained from Eq.(1)

(c) **Low Temperature Simulation**

Perform a new simulation (i.e., all the parts of (b)) at the higher temperature $k_B T = 10.0$. *Hint: Copy and paste is your friend here.*

(d) In the simulations, why do we only take the final 100 time steps, to compute the average spin?

(e) In (b) and (c), how do the theoretical values of $\langle s \rangle$ compare with the computational results? How might we improve the correspondence between the two.

2. **Optional Bonus: MCMC of Mean-Field Ising Model**

Simulate the Mean-Field Ising Model for $J = 1.0$ and *computationally* compute average spin at the two temperature $k_B T = 0.5$ and $k_B T = 1.5$. Compare these computational results with Figure 12(b) in Lecture Notes 05.

Review Problems

(Not to submit)

Preface: This assignment contains a list of review problems to help you prepare for the final exam.

1. **Protein Expression and Probability**

   For a particular model of a gene in a cell, the probability density that said gene produces a concentration of x proteins during the cell cycle is given by

   $$p(x) = A\left(\frac{x}{b}\right)^N e^{-x/b}, \tag{4}$$

   where b is a biological constant with units of concentration and A is a normalization parameter.

   (a) The concentration of proteins that can be produced ranges from zero to infinite. What must A be in order for Eq.(4) to be normalized?

   (b) What is the mean of the normalized probability density?

   (c) What is the standard deviation of the normalized probability density?

2. **Adsorption**

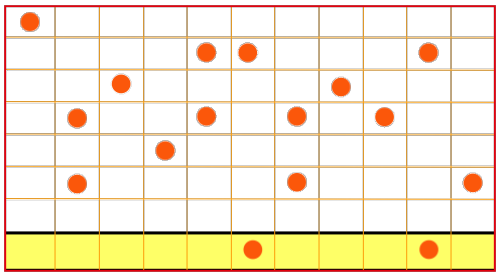

Figure 2: Particular microstate of system. The possible surface states are shown in yellow. The possible bulk states are the remaining states.

A gas is in a container, and some of the atoms are stuck (i.e., "adsorped") to the surface of the container, and others are free to move in the volume. We will study this system using a discrete model of the positions the atoms can take on.

Let M be the number of positions an atom can occupy while in the bulk, and let N be the number of positions an atom can occupy while on the surface. We have N atoms so that the surface states can be completely filled. Let $k \leq N$ be the number of atoms that are on the surface. A *single* atom has energy $-\varepsilon$ while it is on the surface and energy 0 while it is in the bulk. M, N, and ε are all constants, and k is a random variable. M, N, and k are all much greater than 1.

(a) How many microstates does the system have for a particular value of k?

(b) What is the free energy of this system? *You can write this free energy in terms of factorials.*

(c) Use Stirling's approximation $\ln N! \simeq N \ln N - N$ to approximate the result in (b). Derive **one** condition that k must satisfy in order to define the thermal equilibrium of the system. *We often state two conditions associated with thermal equilibrium. Only apply the first-derivative condition.*

3. **Nucleotide zipper**

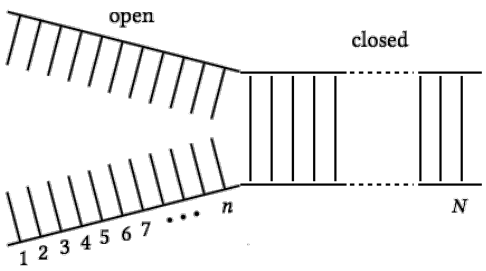

Figure 3: "Zipper" of nucleotides

A strand of DNA can be modeled as a zipper with links between N base-pairs. Each link has the energy 0 in the closed state and the energy ε the open state. Assume the zipper can only open from one end, so that the nth link can open only if all the links $1, 2, ..., n-1$ are open. Assume that the system is at a temperature T.

(a) How many microstates does this system have? What are the energies of these microstates?

(b) Find the partition function for a single DNA strand as a function of T and ε. *Hint: Evaluate the summation using the geometric series identity* $\sum_{n=0}^{N} x^n = (1 - x^{N+1})(1 - x)^{-1}$.

(c) Assume $N \gg 1$. Find the average number of open links as a function of T and ε.

4. **Entropy of an Ideal Gas**
For a system in thermal equilibrium defined by the partition function Z, we determined that the Helmholtz free energy of the system is

$$F = -k_B T \ln Z = -k_B T \ln \sum_{\{i\}} e^{-\beta E_i}, \tag{5}$$

where i denotes a microstate of the system, and E_i is the energy of that microstate.

(a) For a system in thermal equilibrium, the Gibbs entropy is given by

$$S = -k_B T \sum_{\{i\}} p_i \ln p_i = -k_B \sum_{\{i\}} \frac{e^{-\beta E_i}}{Z} \ln \left(\frac{e^{-\beta E_i}}{Z} \right). \tag{6}$$

Given Eq.(5), show that

$$S = -\frac{\partial F}{\partial T}. \tag{7}$$

Note: $\beta = 1/k_B T$.

(b) Using Eq.(7), show that the entropy of an ideal gas for $N \gg 1$ is

$$S \simeq N k_B \left[\ln \left(\frac{V}{N} \right) - \frac{3}{2} \ln \left(\frac{h^2}{2\pi m k_B T} \right) + \frac{5}{2} \right]. \tag{8}$$

Note: You will need to use Stirling's approximation $\ln N! \simeq N \ln N - N$

5. **Partition Function as an Integral**
The partition function for a system of N spins is given by

$$Z(T) = \int_{-\infty}^{\infty} d\rho \, \exp\big[-\beta N f(\rho, T)\big], \tag{9}$$

where

$$f(\rho, T) = -a(T - T_c)\rho^2 + c\rho^4. \tag{10}$$

The parameters a, c, and T_c are constants in the model. T stands in for temperature.

Approximate the partition function using Laplace's method. For what values of T is the approximation invalid?

6. **Transition probabilities and equilibrium probabilities**

A person is in one of four rooms, and after each time step has a probability $1/(M+1)$ of moving to an adjacent room where M is the number of adjacent rooms; The probability of remaining in place is $1/(M+1)$.

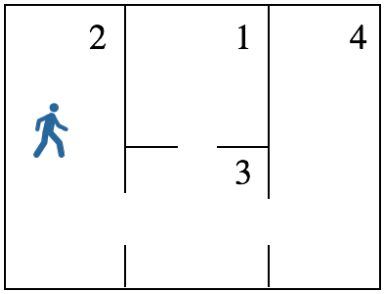

Figure 4: Four connected rooms. The person has a probability $1/(M+1)$ of remaining in place and a probability of $1/(M+1)$ of moving to any one of the adjacent rooms.

(a) Letting $\pi_{i\to j}$ represent the probability of transitioning from room i to room j in a single time step, fill in the elements below

$$\begin{array}{llll} \pi_{1\to1} = & \pi_{1\to2} = & \pi_{1\to3} = & \pi_{1\to4} = \\ \pi_{2\to1} = & \pi_{2\to2} = & \pi_{2\to3} = & \pi_{2\to4} = \\ \pi_{3\to1} = & \pi_{3\to2} = & \pi_{3\to3} = & \pi_{3\to4} = \\ \pi_{4\to1} = & \pi_{4\to2} = & \pi_{4\to3} = & \pi_{4\to4} = \end{array} \tag{11}$$

(b) Using the relationship between equilibrium probabilities and transition probabilities (along with the fact that the equilibrium probabilities are normalized), compute the equilibrium probabilities p_1^{eq}, p_2^{eq}, p_3^{eq}, and p_4^{eq}, to be in rooms 1, 2, 3, and 4.

Resource: Introduction to Statistical Physics

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