Project 2
Numerical Statistical Mechanics

1 Introduction

We investigate a historically important statistical system in physics, the 2D Ising model, using markov chain monte carlo to compute approximate average of physical quantities.

2 Metropolis-Hastings Algorithm

Consider a system with a finite number of states $1, 2, \ldots, N$ with associated probabilities $\pi_1, \pi_2, \ldots, \pi_n$. This means that

$$\sum_{n=1}^{N} \pi_n = 1, \qquad \pi_n \geq 0. \tag{1}$$

An observable O of such a system is a physical quantity that has a certain value o_n if the system occupies state n. The average value of an observable is defined as

$$\langle O \rangle = \sum_{n=1}^{N} p_n o_n. \tag{2}$$

For example, for a system in equilibrium with a heat bath, the the states could be states of definite energy, the probabilities would be the probability of finding the system in one of these states, and the energy itself would be an observable – each state has a certain associated energy value.

It can often be difficult to compute averages of observables for physical systems for various reasons. For example, the system might have an enormous number of states causing naive numerical evaluation of averages to be difficult or impossible. In such cases, a common workaround is to generate a representative random sample $\sigma_1, \sigma_2, \ldots, \sigma_M$ of states and compute the sample average

$$\langle O \rangle_M = \frac{1}{M} \sum_{n=1}^{N} o_{\sigma_n} \tag{3}$$

As M becomes large, the sample average will converge to the average provided the samples are chosen appropriately;

$$\langle O \rangle_M \to \langle O \rangle, \qquad M \to \infty. \tag{4}$$

A powerful method for generating random samples and thus allowing one to compute sample averages is to use a Markov chain to generate a sequence of random samples. This approach is called Markov Chain Monte Carlo (MCMC). In a computational setting, the Markov chain can be generated according to some algorithm. Perhaps the most well-known, simplest, and most elegant of all of these is the so-called **Metropolis-Hastings algorithm**:

1. Initiate the sequence of samples in a state σ_1 of your choosing, and successively generate states in the following way:

2. If σ is the current state, propose a new state σ' according a conditional probability distribution q, namely $q(\sigma'|\sigma)$ is the probability of proposing σ' given the current state is σ.

3. Accept the proposed state, namely add it as the next state in the sample sequence, with probability

$$A(\sigma'|\sigma) = \min\left(1, \frac{\pi_{\sigma'}}{\pi_\sigma}\frac{q(\sigma|\sigma')}{q(\sigma'|\sigma)}\right) \tag{5}$$

   If the state is not accepted, in other words if it is rejected, add the current state σ to your sequence instead as the next state.

4. Repeat these steps for a large number of samples.

The proposal distribution is often chosen to be symmetric

$$q(\sigma|\sigma') = q(\sigma'|\sigma). \tag{6}$$

Choosing this sort of proposal distribution simplifies the acceptance probability to

$$A(\sigma'|\sigma) = \min\left(1, \frac{\pi_{\sigma'}}{\pi_\sigma}\right), \tag{7}$$

and in this case the algorithm is often called simply the **Metropolis algorithm**.

3 Ising Model

The 2D Ising model is a simple model of a ferromagnetic material with a phase transition. The model consists of a 2D lattice $L \times L$ of spins $s_i \in \{-1, +1\}$. Each spin interacts only with its nearest neighbours. The energy is expressed as

$$E(\{s_i\}) = -\sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i, \tag{8}$$

where $\{s_i\}$ is notation for the entire configuration of spins, H is the external magnetic field, and $\langle i, j\rangle$ implies a summation over all nearest-neighbour pairs. We have normalized energy with J, spin with $\hbar/2$, and magnetic field with J/μ, where J is the exchange energy and μ is the atomic magnetic moment. When the system is in contact with a heat bath at temperature T the equilibrium probability density is the Boltzmann distribution

$$\rho(\{s_i\}) = Z^{-1} \exp\big(-E(\{s_i\})/T\big), \tag{9}$$

where the partition function Z is the sum of exponential factors $\exp(-E/T)$ over all possible configurations. Below the critical temperature

$$T_c = \frac{2}{\log(1+\sqrt{2})} \approx 2.2692 \tag{10}$$

the spins are perferentially aligned in a given direction; above T_c the spins have no mean orientation for $H = 0$ (see Fig. 1). One way to implement the Metropolis-Hastings algorithm for the Ising model on a square lattice is the following:

1. Pick a random site i on the 2D lattice and compute the energy change ΔE due to the change of sign in s_i:

$$\Delta E = 2s_i\big(s_{\text{top}} + s_{\text{bottom}} + s_{\text{left}} + s_{\text{right}} + H\big), \tag{11}$$

   where s_{top}, s_{bottom}, s_{left}, and s_{right} are the 4 nearest neighbours of s_i.

2. If $\Delta E \leq 0$ accept the move. If $\Delta E > 0$ accept the move with probability $A = \exp(-\Delta E/T)$.

3. Flip the spin s_i if the move has been accepted.

4. Repeat steps 1-3 until you generate a large sample of spin configurations.

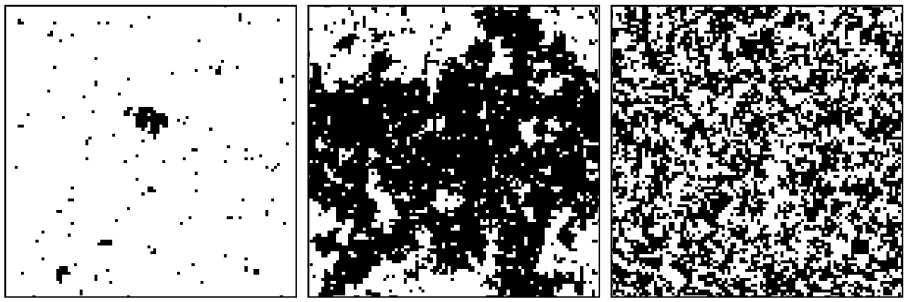

Figure 1: Snapshots of spin configurations in a 2D Ising model on a 100×100 lattice for $T/T_c = 0.7$ (left), $T/T_c = 1$ (middle), and $T/T_c = 1.8$ (right) in the absence of external magnetic field.

4 Assignments

Study the 2D Ising model on square lattice of size $L \times L$ with periodic boundary conditions in the absence of external magnetic field. Determine the dependence of the mean internal energy U, magnetization M, specific heat C_H, and magnetic susceptibility χ_T (per lattice site) on the temperature, where

$$U = \frac{1}{N}\langle E \rangle, \qquad M = \frac{1}{N}\langle S \rangle, \tag{12}$$

$$\chi_T = \frac{1}{NT}\left(\langle S^2 \rangle - \langle S \rangle^2\right), \qquad C_H = \frac{1}{NT^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right), \tag{13}$$

$N = L^2$ is the total number of sites, and $S = \sum_i s_i$ is the net magnetization. Compare the estimate for M with Onsager's exact solution

$$M(T) = \begin{cases} \left[1 - \sinh^{-4}(2/T)\right]^{1/8}, & T < T_c \\ 0, & T \geq T_c \end{cases} \tag{14}$$

obtained in the thermodynamic limit $N \to \infty$. You are welcome to investigate also the effect of a nonzero external field H on the system properties.

We suggest you start the simulations at a high temperature above the critical point T_c and slowly cool the ferromagnet by decreasing the temperature in small steps. After each update of T, perform a large number of iterations with the Metropolis-Hastings algorithm without calculating the ensemble averages. Once the system is close to thermal equilibrium start drawing the samples from the equilibrium distribution and calculate the averages along the way. To save memory, use new samples $\{s_i\}_{n+1}$ immidiately as they arrive to improve your estimates according to the rule

$$\langle O \rangle_{n+1} = \langle O \rangle_n + \frac{1}{n+1}\Big(O\big(\{s_i\}_{n+1}\big) - \langle O \rangle_n\Big),$$

where $\langle O \rangle_n$ is the previous estimate for the mean of some observable O obtained from a sequence of n samples, and $\langle O \rangle_{n+1}$ is the new improved estimate. Avoid also updating the energy and magnetization by looping over all sites of the $L \times L$ lattice. It is necessary to perform this time-consuming operation only once at the very start of the simulation. Afterwards you can keep track of E and S by adding the increments ΔE and Δs to the old values.