

## STAT 576 HOMEWORK 4

DUE DEC. 13, 2024 (FRIDAY), 11:59 PM PST

NOTES. **NO** late submission will be accepted except for approval from the instructor. Answers should be either scanned or typed. For the coding part (if any), you may either prepare an R notebook or put the code in a separate file.

### 2D Ising Model

In this homework, we will investigate the phase transition phenomenon in the 2D Ising model through Markov Chain Monte Carlo. The 2D Ising system consists of a lattice of spins  $s_{ij} \in \{-1, 1\}$ , where  $i = 1, \dots, m$  and  $j = 1, \dots, n$ . The energy of the system is given by

$$E(\mathbf{s}) = -J \sum_{i,j} \sum_{(i',j') \in \mathcal{N}_{ij}} s_{ij} s_{i'j'},$$

where  $\mathcal{N}_{ij}$  is the set of nearest neighbors of  $(i, j)$ , and  $J$  is the coupling constant. For example, if  $(i, j) = (3, 3)$ , then  $\mathcal{N}_{33} = \{(2, 3), (4, 3), (3, 2), (3, 4)\}$ . If  $(i, j) = (1, 2)$ , then  $\mathcal{N}_{12} = \{(1, 1), (1, 3), (2, 2)\}$ . This energy contains all the pairwise interactions between the spins.

The distribution of the spins is given by the Boltzmann distribution

$$p_T(\mathbf{s}) \propto \exp \left\{ -\frac{E(\mathbf{s})}{kT} \right\},$$

where  $T$  is the temperature and  $k$  is the Boltzmann constant. The average magnetization is given by

$$\mathcal{M}(T) = \left| \mathbb{E}_{p_T} \left[ \frac{1}{mn} \sum_{i,j} s_{ij} \right] \right|$$

is the average spins of the system under the Boltzmann distribution at temperature  $T$ .

- For simplicity, we set  $k = 1$  and  $J = 5$ . What is the conditional distribution of  $s_{ij}$  given all the other spins?
- For  $m = n = 16$  and  $T = 5$ , write a MCMC program to sample from the Boltzmann distribution and estimate the average magnetization  $\mathcal{M}_5$ . (Hint: you can use the Gibbs sampler to sample from the distribution.)
- It is a well-known fact that the 2D Ising model exhibits a phase transition at some critical temperature  $T_c$ . The average magnetization  $\mathcal{M}(T)$  is expected to be zero for  $T > T_c$  and non-zero for  $T < T_c$ . Repeat part (b) for different temperatures between  $T = 1$  and  $T = 25$  and plot the average magnetization as a function of temperature. What do you observe?