Stochastic Simulations

Autumn Semester 2020

Prof. Fabio Nobile *Assistants: Juan Pablo Madrigal Cianci*

Homework 2: Due date: 02 December 2020

Homework 2: Markov chain Monte Carlo

The following problem is optional and counts for a bonus of up to 0.2 points in the final grade.

Let us consider a 2D uniform square-lattice with atoms placed at each vertex, as is sketched in Figure 1. The atoms can have an upward (red arrow) or a downward (blue arrow) pointing

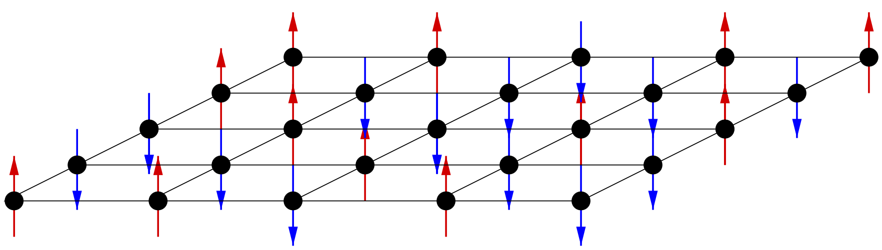

Figure 1: Sketch of 2D square-lattice Ising model.

magnetic moment (so-called *spin*). Specifically, let the lattice be made out of $m \times m$ atoms. Therefore the system's possible states are the 2^{m^2} possible spin choices for the m^2 atoms. That is, the spin of the atom at position (i, j) in the lattice is denoted with s_{ij}, $1 \leq i, j \leq m$, and can take a value in $\{-1, +1\}$. A specific system configuration is described by the matrix $\boldsymbol{S} = (s_{ij}) \in \{-1, +1\}^{m \times m}$, containing the spin of each of the m^2 atoms.

The energy of a given system state of this Ising model is given by

$$H(\boldsymbol{S}) = -\sum_{i,j=1}^{m} \left(\frac{1}{2} J s_{ij} (s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}) + B s_{ij} \right) , \tag{1}$$

where J is a magnetic coupling constant and B is a constant describing the external magnetic field. To account for boundary effects, we set $s_{0,j} = s_{j,0} = s_{m+1,j} = s_{j,m+1} = 0$ in (1). That is, the energy defined in equation (1) only accounts for the interactions between neighboring atoms. The probability of obtaining a specific system state is then given by the *Boltzmann* distribution with probability mass function (PMF)

$$f(\boldsymbol{S}) \equiv f_\beta(\boldsymbol{S}) = \frac{1}{Z_\beta} e^{-H(\boldsymbol{S})\beta} , \tag{2}$$

where $\beta = 1/(k_B T)$ denotes the so-called inverse-temperature (or thermodynamic beta) with k_B being the Boltzmann constant and T the absolute temperature. Here, Z_β denotes the normalization constant that makes the target distribution $f_\beta \colon \{-1,+1\}^{m\times m} \to \mathbb{R}_+$ a proper PMF.

Let's denote by $M(\boldsymbol{S}) = \sum_{ij} s_{ij}$ the system's total magnetic moment corresponding to the configuration $\boldsymbol{S}$. Notice that the random realizations of the configuration matrix $\boldsymbol{S}$ depend on the inverse temperature β. The expected value of the total magnetic moment as a function of the inverse temperature thus reads

$$\bar{M}(\beta) = \sum_{\boldsymbol{S}\in\mathcal{K}} M(\boldsymbol{S}) f_\beta(\boldsymbol{S}) = \frac{1}{Z_\beta} \sum_{\boldsymbol{S}\in\mathcal{K}} M(\boldsymbol{S}) e^{-H(\boldsymbol{S})\beta} \,, \tag{3}$$

where $\mathcal{K} = \{-1,1\}^{m\times m}$ is the set of all possible system configurations. Since the explicit computation of the normalization constant Z_β is computationally expensive for even moderate values of m (Explain why!), we rely on the Metropolis–Hastings algorithm here. That is, at each step a candidate configuration is proposed by randomly choosing an atom, with uniform probability, and "flipping" its spin.

1. Write a `Python` function that implements the Metropolis–Hastings algorithm for the Ising model. The input parameters for your function are: the number of steps n of the chain that should be simulated, the number of atoms m, the inverse temperature β, the constants J and B, and the initial state of the system. The function should return a list of energies and total magnetic moments computed for each step of the chain, as well as the final configuration of the system.

2. Use your `Python` function with $\beta = 1$ and for n, such that both the energy and the total magnetic moment appear to have reached a stationary state. Plot also the final system configuration. Furthermore, compute the mean total magnetic moment $\bar{M}(\beta)$ for different values of $\beta \in [\frac{1}{3}, 1]$ and $n = 5 \cdot 10^6$. Choose a lattice of 50×50 atoms, $J = 1$, and $B = 0$ for all simulations.

3. Set $m = 4$ and compute the exact expected value of the total magnetic moment $\bar{M}(\beta)$ using (3). Run your MH algorithm for the Ising model (with $m = 4, J = 1, B = 0, \beta = 1/3$), compute the total magnetic field with the samples obtained, and estimate its convergence to the true $\bar{M}(\beta)$ as a function of the number of samples n.