Homework #5
Math 589B

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Problem 25.1. *Using Metropolis algorithm, simulate a Markov chain with* $P(x) = exp(-x), x \geq 0$ *density and transition function* $T(x'|x) = exp(-(x'-x)^2/2\sigma^2)/\sqrt{2\pi}\sigma$ *(with appropriate acceptance probability* $A(x'|x)$*). Find* σ *that minimizes* $K_{xx}(1) = \mathbb{E}(x_m - 1)(x_{m-1} - 1)$*, where* x_m *is the state of the Markov chain at time* m*.*

Solution. For the function that simulates a Markov chain, please refer to code.

We simulate for the best σ that minimizes the autocorrelation and find that $\sigma = 2.42$ is the most optimal choice.

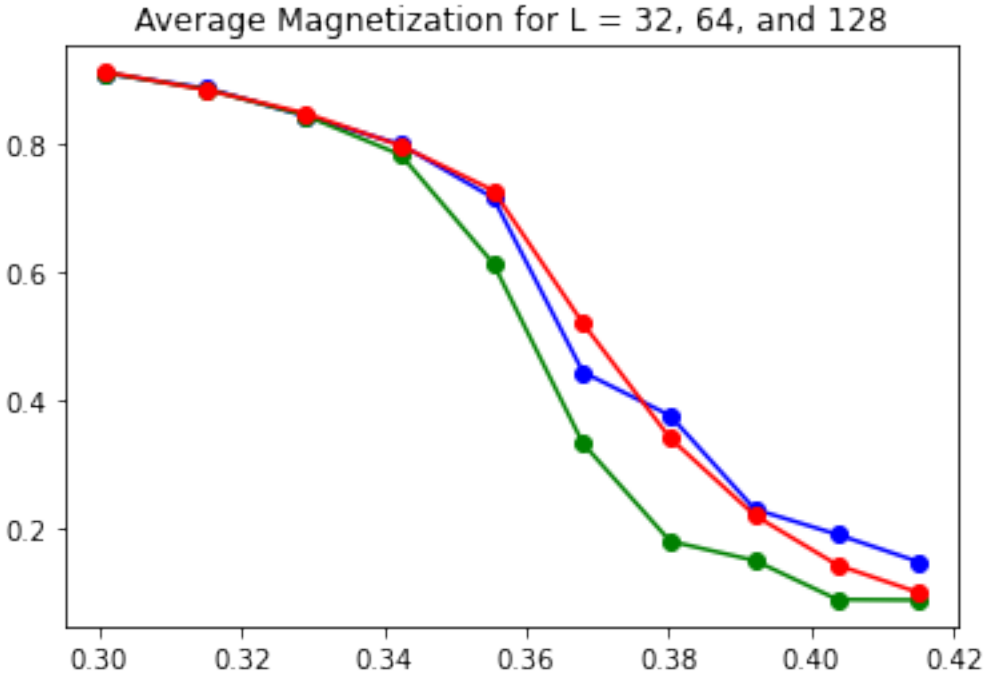

Figure 1: Average Magnetization for $L = 32$, 64, and 128 as a function of T, $2 \leq T \leq 2.6$. The blue, green and red lines denote the average values for $L = 32$, 64, and 128 respectively. Here, the x-axis is given in terms of log-scale.

Problem 25.2. *Using either Metropolis algorithm or Glauber dynamics, simulate a MCMC for 2D Ising model on a $L \times L$ torus of binary variables/spins. Compute and plot as a function of temperature T (e.g, for $2 \leq T \leq 2.6$) the average value of $m(T) = |\sum_n \sigma_n|/L^2$ for $L = 32, 64$, and 128. Does the transition from non-zero to [almost] zero value of $m(T)$ become sharper for larger L?*

Solution. We plot the average magnetization over the interval $[2, 2.6]$. See Figure 1 for the plot, with x-axis given in log-scale. From the plot, we find that the transition to almost zero magnetization becomes sharper as a function of L.

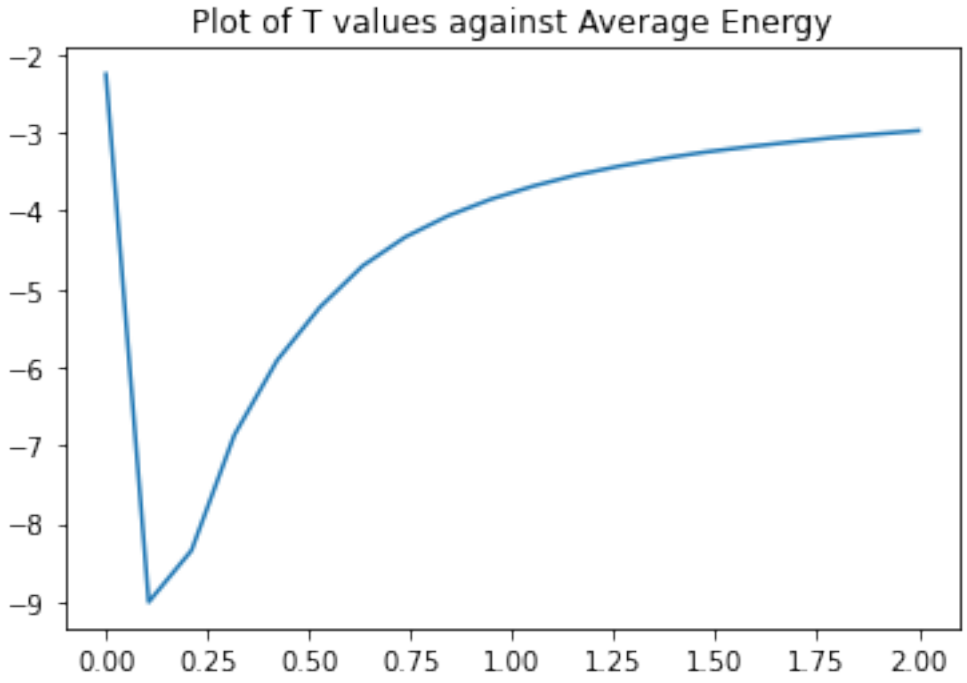

Figure 2: Plot of Average Energy Values as a Function of Temperature

Problem 25.3. *There are $N = 10$ particles that occupy discrete sites in a ring of length $L = 40$. (See the picture). No 2 particles may occupy the same site. One can represent the state, e.g. by the coordinates of the particles $0 \le x_n \le L$, with $1 \le n \le N$. In this case $x_m \ne x_n$ whenever $m \ne n$. Another way to represent the state is the set of numbers n_x, where $0 \le x < L$, which are equal to either 0 (no particle at site x) or 1 (there is a particle at site x). The energy of the state is equal to minus the number of neighboring pairs of particles (here n_L is used as an alias for n_0):*

$$E\{\boldsymbol{x} \text{ or } \boldsymbol{n}\} = -\sum_{x=0}^{L-1} n_x n_{x+1} = -\sum_{m=1}^{N}\sum_{n=1}^{N} \delta_{x_m - x_n, 1(mod\ L)} = -\sum_{m=1}^{N-1}\sum_{n=m+1}^{N} \begin{cases} 1, & |x_m - x_n| = 1 \\ 0, & |x_m - x_n| \ne 1 \end{cases} \tag{1}$$

The distribution over states is $\mathbb{P}(state) = exp(-E(state)/T)/Z(T)$, where T is temperature and $Z(T) = \sum_{state} exp(-E(state)/T)$ is the partition sum (for normalization). Plot the average energy $\langle E \rangle = \sum_{state} E(state)\mathbb{P}(state)$ as a function of temperature T (e.g. for $0 \le T \le 2$).

Solution. We plot the average energy as a function of temperature. See Figure 2.