Markov Chain Monte Carlo approximation of the infinite lattice Ising model

Alessio Canclini, Filip von der Lippe (Dated: November 4, 2022)

NB! Abstract here

I. INTRODUCTION

This report will explore temperature-dependent behavior in ferromagnetism using the two-dimensional **Ising model**. The main purpose is determining a numerical estimation of the **critical temperature** at which the system transitions from a magnetized to a non-magnetized phase.

 \dots more about Ising model and phase transitions + Mote Carlo methods and Markov chains.

II. METHODS

The square 2D lattices for our Ising model will have a length of L containing N spins with the relation $N = L^2$. Each spin s_i will have two possible states of

$$s_i = -1 \text{ or } s_i = +1.$$
 (1)

The total spin state or **spin configuration** of a lattice will be represented as $\mathbf{s} = (s_1, s_2, ..., s_N)$. The following equations will be used:

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l \tag{2}$$

E is the total energy where $\langle kl \rangle$ denotes the sum going over all neighboring pairs of spins avoiding double-counting. J is the **coupling constant** simply setting the energy associated with spin interactions. Periodic boundary conditions will be implemented allowing all spins to have four neighbors.

$$M(\mathbf{s}) = \sum_{i}^{N} s_i \tag{3}$$

Here M is the magnetization of the entire system expressed as a sum over all spins.

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N} \tag{4}$$

$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N} \tag{5}$$

 ϵ is the energy per spin and m the magnetization per spin. These will be used to compare results.

$$\beta = \frac{1}{k_B T} \tag{6}$$

 β describes the "inverse temperature" with the systems' temperature T and the Boltzmann constant k_B .

$$Z = \sum_{\text{all possible } \mathbf{s}} e^{-\beta E(\mathbf{s})} \tag{7}$$

Z is the partition function. This, the 'inverse temperature" and the total energy of the system appear in the $Boltzmann\ distribution$ given bellow.

$$p(\mathbf{s};T) = \frac{1}{Z}e^{-\beta E(\mathbf{s})} \tag{8}$$

For comparison with early numerical implementations we will fist consider an analytical solution. The following table I summarizes all sixteen possible **spin configurations** of a 2×2 lattice with *periodic boundary conditions*.

TABLE I. Analytic values for the sixteen spin configurations of 2×2 Ising model lattice.

	0		
Nr. of spins	s Total	Total	Degeneracy
in state $+1$	energy	magnetization	Degeneracy
0	-8	-4	1
1	0	-2	4
1	0	-2	4
1	0	-2	4
1	0	-2	4
2	0	0	4
2	0	0	4
2	8	0	2
2	0	0	4
2	0	0	4
2	8	0	2
3	0	2	4
3	0	2	4
3	0	2	4
3	0	2	4
4	-8	4	1

Based on the values in table I we derive the specific analytical expressions bellow for the 2×2 lattice case.

III. RESULTS

IV. DISCUSSION

V. CONCLUSION