# ONE- AND TWO-DIMENSIONAL ISING MODEL

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## 1. Introduction

A large number of systems change their macroscopic properties at thermal equilibria. For example magnetic atoms align them selves to form a magnetic material at low temperature or high pressure. When modeled mathematically, these phase transitions only occur in infinitely large systems [3]. This paper investigates a simulation of a finite system, the Ising ferromagnet to be exact.

Section 1.1 introduces the Ising model of ferromagnetism, the next section discusses the Metropolis Monte Carlo method that is used to estimate the Ising model numerically.

## 1.1. Ising Model

A magnet can be modeled as a large collection of electronic spins. In the Ising model spins point either up, s = +1, or down, s = -1 [8]. At high temperatures the spins point in random directions, consequently the magnetization is approximately zero. At a low enough temperature all spins in the two-dimensional model align themselves, this effect is called spontaneous magnetization. The temperature at which this phase transition occurs is called the critical temperature,  $T_c$  [1]

Section 1.1.1 and 1.1.2 introduce the oneand two-dimensional Ising model, respectively.

#### 1.1.1. One-Dimensional Model

Ising [2] introduced a model consisting of a one-dimensional lattice op spin variables. Contrary to the two dimensional model this model does not exhibit state transitions. The Hamiltonian of the one dimensional Ising model with the set spins  $\mathcal{S} = \{s_1, \ldots, s_N\}$  is

$$\mathcal{H}(\mathcal{S}) = -\mathcal{J}\sum_{\langle i,j\rangle} \mathbf{s}_{i}\mathbf{s}_{j} - \mathbf{h}\sum_{i} \mathbf{s}_{i}. \tag{1}$$

Where  $\langle i,j \rangle$  is a nearest neighbour pair, the nearest neighbour of  $\mathbf{S}_i$  in the one dimensional model are  $\mathbf{S}_{i-1}$  and  $\mathbf{S}_{i+1}$ .  $\mathcal{J}$  specifies the strength of the interactions between the particles. In a ferromagnetic model,  $\mathcal{J} > 0$  neighboring spins prefer to be parallel. In the anti-ferromagnetic model,  $\mathcal{J} < 0$  spins prefer a direction different to one of their neighbors. The constant h represents the external magnetic field, the spins want to align with the direction of h, i.e. when h > 0 spins prefer to be positive.

In the following the zero-field ferromagnetic model, i.e.  $\mathcal{J} = 1$  and h = 0, is considered. The energy E of a configuration of spins,  $\mathcal{S}$ , in this model is given by

$$E\left(\mathcal{S}\right) = \sum_{n=1}^{N-1} s_n s_{n+1}.$$

The probability of realising a configuration of spins S with energy E is given by

$$P(S) = \frac{1}{Z} \exp\left[-E(S)\frac{1}{T}\right],$$
 (2)

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where T represents the temperature,  $\beta = {}^{1}/_{T}$  and Z is the partition function:

$$Z = \sum_{\{s_1, \dots, s_N\}} \exp\left[-E(\mathcal{S})\beta\right]. \tag{3}$$

Both the one and two dimensional Ising model can be solved analytically. Under free end boundary conditions, i.e. the boundary particles,  $s_1$  and  $s_N$ , only observe one neighbor [5], the analytical solution of equation (3) is

$$Z = (2\cosh\beta)^{N}.$$
 (4)

The average energy can be expressed as a function of Z [6]

$$U = \frac{1}{Z} \cdot \sum_{S_{i} \in \Phi} E(S_{i}) \cdot \exp\left[-\beta E(S_{i})\right],$$

where  $\Phi$  is the set of all possible configurations, i.e.  $\Phi = \{S_1, \dots, S_{2^N}\}$ . Observing that

$$\frac{\partial Z}{\partial \beta} = \sum_{S_i \in \Phi} -E\left(S_i\right) \exp\left[-\beta E\left(S_i\right)\right],$$

and by following the steps presented in appendix A.1 it can be found that

$$U = -\frac{\partial \ln [Z]}{\partial \beta} = -\mathbf{N} \cdot \tanh(\beta).$$

Consequently  $U/N = -\tanh(\beta)$ .

The specific heat describes how the average energy changes as a function of the temperature. Consequently

$$C = \frac{\partial U}{\partial T} = N \left( \frac{\beta}{\cosh(\beta)} \right)^2$$

as shown in appendix A.2 [9], consequently

$$\frac{C}{N} = \left(\frac{\beta}{\cosh(\beta)}\right)^2.$$

#### 1.1.2. Two-Dimensional Model

The 2D Ising model is a square lattice whose lattice sites are occupied by spins. Each spin has either a positive or a negative spin [3].

The Hamiltonian of the 2D model is the same as the one of the one dimensional model given in equation (1). The pairs of nearest neighbours are now found by looking at the four connected neighbours, i.e. the nearest neighbours of spin  $S_{i,j}$  are  $S_{i-1,j}$ ,  $S_{i+1,j}$ ,  $S_{i,j-1}$  and  $S_{i,j+1}$ . The energy of a configuration  $S_n$  that has  $d \times d$  spins is computed as

$$E(S_n) = -\sum_{i=1}^{d-1} \sum_{j=1}^{d} S_{i,j} S_{i+1,j}$$

$$-\sum_{i=1}^{d} \sum_{j=1}^{d-1} S_{i,j} S_{i,j+1}.$$
(5)

The two-dimensional Ising model has been solved analytically by Onsager [7]. He showed that the average magnetization per spin on a infinite 2D lattice, i.e.  $N = \infty$ , is

$$\frac{M}{d^2} = \begin{cases} (1 - \sinh^{-4}(2\beta))^2 & \text{if } T < T_c \\ 0 & \text{if } T > T_c \end{cases}$$
 (6)

where

$$T_c = \frac{2}{\ln\left(1 + \sqrt{2}\right)}.$$

Given equation (3) solving the the Ising model is relatively simple. To find which configurations of spins result in an equilibirium one only needs to try them all. Unfortunately the computational complexity of this operation is exponential in N, the number of spins. To be exact, a lattice with N spins has  $2^{N}$  possible configurations, computing E according to equation (5) for one configuration takes  $2^{N}$  steps. This leads to  $2^{N}$  computation steps [3]. Solving the problem with the Metropolis Monte Carlo method circumvents this complexity problem.

#### 1.2. Metropolis Monte Carlo

Monte Carlo methods rely on random sampling to obtain numerical results. They are often used to solve problems that might be deterministic in principle but are difficult to solve with other approaches. Monte Carlo experiments can be used for sampling, i.e. generating draws from some probability distribution [4].

In the context of the Ising model one could naively consider using a few randomly generated states to compute the partition function. However the central limit theorem tells us that randomly generated states have an energy that is approximately  $\mathcal{O}(\sqrt{N})$  for sufficiently large N. However the states that we are interested in have an energy of the order  $\mathcal{O}(N)$ , which means that they are not generated at all by the naive method.

Consequently we need some way to generate the physically relevant states. This can be done by relaxing some configuration into a thermal equilibrium by generating from it a new sequence of states. This requires a transition probability  $W(S_i \to S_j)$  from configuration  $S_i$  to configuration  $S_j$ . In thermal equilibrium the probability of finding a given configuration is presented in equation (2). As we require  $P(S_i)$  to be stationary in thermal equilibrium we get the detailed balance:

$$W(S_i \to S_j) \exp[-E(S_i)\beta] = W(S_j \to S_i) \exp[-E(S_j)\beta]. \quad (7)$$

The function  $W(\cdot)$  needs to cover the entire configuration space. The Metropolis algorithm is one of the algorithms that ensures this [3].

The Metropolis Monte Carlo algorithm starts in some initial configuration, it then moves to subsequent configurations by flipping one randomly selected spin with a probability defined by  $W(\cdot)$ . This is repeated for a given number of steps.

Section 2 discusses how the Metropolis Monte Carlo method was used to solve the Ising model. In section 3 the run experiments are introduced, their results are presented in section 4. Section 5 discusses the found results and section 6 concludes this paper.

## 2. Method

Algorithm 1 presents the pseudo code of the Metropolis Monte Carlo algorithm applied to the Ising problem. This section starts by discussing the input of this algorithm and then introduces the functions used in algorithm 1 one by one. It should be noted that the discussed algorithm is agnostic to the dimensionality of the model.

## Algorithm 1: $MMC(S_{init}, N_{iterations})$

input :  $S_{init}$  the initial configuration  $N_{iterations} \text{ number of iterations}$ 

```
egin{aligned} \mathcal{S}_{cur} &:= \mathcal{S}_{init} \ & 	ext{for } i = 0 	ext{ to } N_{iterations} 	ext{ do} \ & 	ext{S} := 	ext{selectRandomSpin}\left(\mathcal{S}_{cur}
ight) \ & \mathcal{S}_{pot} := 	ext{flipSpin}\left(	ext{s}, \ \mathcal{S}_{cur}
ight) \ & \mathcal{S}_{cur} := 	ext{selectConfig}\left(\ \mathcal{S}_{cur}, \ \mathcal{S}_{pot} \ 
ight) \end{aligned}
```

Algorithm 1 requires an initial configuration  $S_{init}$  as input, this configuration is a representation of the system in its initial state. The parameter  $N_{iterations}$  indicates how many configurations are generated, generally  $N_{iterations} = N$ . Before the start of the first loop the the current configuration is set to the initial configuration.

selectRandomSpin() selects on spin randomly from the spins in  $\mathcal{S}_{cur}$ . The potential configuration,  $\mathcal{S}_{pot}$  is a copy of  $\mathcal{S}_{cur}$  with the selected spin, s, flipped. This new configuration is generated by flipSin(). The new current configuration is selected by selectConfig(). The pseudo code of this function is presented in algorithm 2.

Given two configurations,  $S_{pot}$  and  $S_{cur}$ , selectConfig() selects with which one the simulation should continue. To this end  $\Delta E$ , the difference in energy between the two configurations, is computed. It is not possible to compute the energy of the two configurations according to equation (5). However writing

# Algorithm 2: selectConfig( $S_{cur}, S_{pot}$ )

input :  $S_{cur}$  the current configuration  $S_{pot}$  the potential configuration

**output**:  $S_{new}$  the selected configuration

 $\Delta E := ext{computeDeltaE} ( \ \mathcal{S}_{cur}, \ \mathcal{S}_{pot} \ )$ 

 $\xi := \exp\left[-\beta \Delta E\right]$ 

 $\theta := randomNumber(0, 1)$ 

if  $\xi > \theta$  then  $S_{new} := S_{pot}$ 

else  $S_{new} := S_{cur}$ 

equation (1) as

$$\mathcal{H}(\mathcal{S}) = -\mathbf{S}_{i} \sum_{j \in \mathcal{N}(\mathbf{S}_{i})} \mathbf{S}_{j} + remainder \quad (8)$$

where  $\mathcal{N}(s_i)$  is the neighborhood of  $s_i$  allows us to see that since only  $s_i$  changes the remainder of  $\mathcal{H}(\mathcal{S}_{cur})$  and  $\mathcal{H}(\mathcal{S}_{pot})$  are the same [3]. Thus only the first term in equation (8) is relevant for the computation of  $\Delta E$ , consequently we find:

$$\Delta E = -2 \cdot \mathbf{s}_i \sum_{j \in \mathcal{N}(\mathbf{s}_i)} \mathbf{s}_j. \tag{9}$$

If a the potential configuration is determined is decided by two values:  $\theta$  and  $\xi$ . The first is sampled from a pseudo random uniform distribution with the range (0,1). The second is computed from  $\Delta E$  according to

$$\xi = \exp\left[-\beta \Delta E\right]. \tag{10}$$

If the transition from  $S_{cur}$  to  $S_{pot}$  decreases the energy of the system  $\xi$  is greater than one and as  $\theta \in (0,1)$  potential states with an energy that is lower than that of the current state are always accepted. The guard of the if also ensures that state transitions that increase the energy, i.e.  $\xi < 1$ , are not necessarily discarded.

The implementation of the presented algorithm can be found in listings 1 to 3 in appendix C.1.

### 3. Experiments

This section introduces the experiments we ran with the model introduced in the previous sections. In the experiments below the number of iterations,  $N_{iterations}$ , is not necessarily equal to N, the number of spins, but set independently. To give the system time to relax into the interesting states we perform  $^{1}/_{10} \cdot N_{iterations}$  Monte Carlo steps, before actually taking the samples used to compute the results.

The experiments we ran with the one and two dimensional model are discussed in sections 3.1 and 3.2, respectively.

#### 3.1. One-Dimensional Model

In the 1D model we are interested in both the average energy and the specific heat per spin in the following parameter space  $T = 0.2, 0.4, \dots, 4$ , N = 10, 100, 1000 and  $N_{iterations} = 1000, 10000$ .

U, the average energy is given by

$$U = \frac{1}{\#\Omega} \sum_{S_i \in \Omega} E(S_i), \tag{11}$$

where  $\Omega = \left\{ S_1, \dots, S_{N_{samples}} \right\}$  is the set of configurations generated during the Monte Carlo steps. C, the specific heat is defined as

$$C = \beta^2 \left( \frac{1}{\#\Omega} \left( \sum_{\mathcal{S}_i \in \Omega} E^2(\mathcal{S}_i) \right) - U^2 \right). \tag{12}$$

Furthermore we will compare the results of the simulation with the analytical solution presented earlier. To compare the numerical and analytical results the mean accuracy of the specific heat and the average energy per spin are computed. The accuracy of a variable where  $\nu$  and  $\alpha$  represent the numerically and analytically found values, respectively is

$$accuracy = 1 - \left| \frac{|\nu - \alpha|}{\alpha} \right|. \tag{13}$$

The discussed experiment is implemented in listing 8. The implementation of equations (11) to (13) are presented in listings 4 to 6, respectively. All mentioned listings can be found in appendix C.

#### 3.2. Two-Dimensional Model

In the 2D model we are not only interested in the average energy and specific heat per spin but also the average magnetization per spin. The magnetization of a magnet in the Ising model can be computed according to:

$$M = \frac{1}{\#\Omega} \sum_{S_i \in \Omega} \sum_{S_j \in S_i} S_j.$$
 (14)

The following parameter space is used:  $T = 0.2, 0.4, \ldots, 4$ , d = 10,50,100 and  $N_{iterations} = 1000,10000$ . The found average average magnetization per spin is compared with the analytical solution presented in equation (6).

The discussed experiment and equation (14) are presented in listings 7 and 9 in appendix C, respectively.

## 4. Results

This section presents the results of the experiments with the one- and two- dimensional model discussed in section 3, in section 4.1 and section 4.2, respectively.

#### 4.1. One-Dimensional Model

Tables 1 to 6 in appendix B present the results of the experiment with the one dimensional model.

In tables 1 and 2 we observe that the accuracy of the 1D simulation is reasonable for temperatures greater than 0.4. In the simulation with N = 10. The simulation with N = 100 starts being accurate at T=1.4 if  $N_{samples}=1000$  and at T=0.8 if  $N_{samples}=10000$ . If we increase the number of particles to N = 1000 we only find reasonable accuracy with  $N_{samples}=10000$  for T>1.6.

For all values of N we find that the accuracy improves in general as the number of samples increases, although this effect is stronger in simulations with more spins.

#### 4.2. Two-Dimensional Model

The average energy, specific heat and average magnetization per spin for the different combinations of N and  $N_{samples}$  can be found in figure 1.

### 5. Discussion

What are we going to discuss?

Interpret results in terms of a phase transition from a state with magnetization zero to a state with definite magnetization (slide 31)

Invloed van de parameters, T, N, NSAM-PLES p 192 physics by computer

#### 5.1. One-Dimensional Model

Compare results with the analytical solution

## 5.2. Two-Dimensional Model

Compare Average magnetization with the exact result for the infinite system

### 6. Conclusion

Hoe goed sluit het model aan bij de het exacte resultaat?

Wat hebben we geleerd over de parameters.

./img/2D/averageEnergy.pdf

(a) Average energy per spin.

./img/2D/specificHeat.pdf

(b) Average magnetization per spin.

./img/2D/averageMagnetization.pdf

(c) Average magnetization per spin.

Figure 1: The (a) average energy, (b) specific heat and (c) average magnetization per spin in a 2D Ising model with d=10,50,100 and  $N_{samples}=1000,10000$ .

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## A. MATHEMATICAL DERIVATIONS

## A.1. Average Energy<sup>1</sup>

$$\begin{split} U &= & -\frac{\partial \ln{[Z]}}{\partial \beta} \\ &= \left\{ Definition \ of \ Z \ in \ equation \ (4). \right\} \\ &- \frac{\partial \ln{\left[ (2\cosh{\beta})^N \right]}}{\partial \beta} \\ &= \left\{ Chain \ rule: \ \frac{\partial}{\partial \beta} \ln{\left[ 2^N \cosh^N(\beta) \right]} = \frac{\partial \ln{[u]}}{\partial u} 0, \ u = 2^n \cosh^n(\beta), \ \frac{\partial}{\partial u} \ln{[u]} = \frac{1}{u} \right\} \\ &- 2^{-N} \cosh^{-N}(\beta) \left( \frac{\partial}{\partial \beta} \left( 2^N \cosh^N(\beta) \right) \right) \\ &= \left\{ Factor \ out \ constants. \right\} \\ &- 2^{-N} \frac{\partial}{\partial \beta} \left( \cosh^N(\beta) \right) 2^N \cosh^{-N}(\beta) \\ &= \left\{ Simplify \ the \ expression. \right\} \\ &- \cosh(\beta)^{-N} \left( \frac{\partial}{\partial \beta} \cosh^N(\beta) \right) \\ &= \left\{ Chain \ rule: \ \frac{\partial}{\partial \beta} \cosh^N(\beta) = \frac{\partial u^N}{\partial u} 0, \ u = \cosh(\beta), \ \frac{\partial}{\partial u} \left( u^N \right) = N \cdot u^{-1+N} \right\} \\ &- N \cosh(\beta)^{N-1} \frac{\partial}{\partial \beta} \left( \cosh(\beta) \right) \cosh^{-N}(\beta) \\ &= \left\{ Simplify \ the \ expression. \right\} \\ &- N \left( \frac{\partial}{\partial \beta} \cosh(\beta) \right) \operatorname{sech}(\beta) \\ &= \left\{ Derivative \ of \ \cosh(\alpha) \ is \ \sinh(\alpha). \right\} \\ &- \sinh(\beta) N \operatorname{sech}(\beta) \\ &= \left\{ Simplify \ the \ expression. \right\} \\ &- N \tanh(\beta) \end{split}$$

### A.2. Specific Heat

$$\begin{split} C &= \frac{\partial U}{\partial T} \\ &= \{ Definition \ of \ specific \ heat. \} \\ &= \frac{\partial U}{\partial \beta} \cdot \frac{1}{\partial T} \\ &= \{ Derivate \ of \ T \ w.r.t. \ to \ \beta. \} \end{split}$$

<sup>&</sup>lt;sup>1</sup>The derivation has been computed with Wolfram Research, Inc. [10].

$$\begin{split} &\frac{\partial U}{\partial \beta} \cdot \frac{1}{^{-1/}_{\beta^2}} \\ &= \{Rewrite.\} \\ &- \beta^2 \frac{\partial U}{\partial \beta} \\ &= \{Definition \ of \ U.\} \\ &- \beta^2 \left(\frac{\partial}{\partial \beta} - N \tanh(\beta)\right) \\ &= \left\{\frac{\partial}{\partial \beta} - N \tanh(\beta) = -N \frac{\partial}{\partial \beta} \tanh(\beta) = -N \operatorname{sech}^2(\beta)\right\} \\ &\beta^2 N \operatorname{sech}^2(\beta) \\ &= \left\{Definition \ of \ \operatorname{sech}(\alpha) = \frac{1}{\cosh(\alpha)}.\right\} \\ &N \left(\frac{\beta}{\cosh(\beta)}\right)^2 \end{split}$$

# B. Results

**Table 1:** Results of the 1D simulation for N=10,  $N_{samples}=1000$ .

		Numerical		Analytical		
T	$\beta$	$U_{/N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
0.20	5.00	-0.900	0.	-1.000	0.004 54	$-\infty$
0.40	2.50	-0.900	0.00250	-0.987	0.166	-32
0.60	1.67	-0.833	0.421	-0.931	0.370	0.88
0.80	1.25	-0.771	0.450	-0.848	0.438	0.94
1.0	1.00	-0.707	0.419	-0.762	0.420	0.96
1.2	0.833	-0.643	0.269	-0.682	0.371	0.78
1.4	0.714	-0.538	0.241	-0.613	0.318	0.77
1.6	0.625	-0.467	0.223	-0.555	0.270	0.80
1.8	0.556	-0.432	0.248	-0.505	0.230	0.88
2.0	0.500	-0.428	0.198	-0.462	0.197	0.96
2.2	0.455	-0.369	0.137	-0.426	0.169	0.81
2.4	0.417	-0.343	0.131	-0.394	0.147	0.86
2.6	0.385	-0.316	0.124	-0.367	0.128	0.91
2.8	0.357	-0.312	0.106	-0.343	0.113	0.92
3.0	0.333	-0.321	0.0754	-0.322	0.0996	0.84
3.2	0.313	-0.291	0.0926	-0.303	0.0887	0.96
3.4	0.294	-0.292	0.0824	-0.286	0.0794	0.97
3.6	0.278	-0.234	0.0593	-0.271	0.0715	0.82
3.8	0.263	-0.227	0.0563	-0.257	0.0647	0.86
4.0	0.250	-0.203	0.0520	-0.245	0.0588	0.83

Table 1: continued

		Numerical		An	alytical	
T	$\beta$	$U_{\rm N}$	$C_{/N}$	$U_{/N}$	$^{C}$ / $_{ m N}$	accuracy

Table 2: Results of the 1D simulation for N = 10,  $N_{samples}$  = 10000.

		Numerical		Analytical		
T	$\beta$	$U_{/N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
0.20	5.00	-0.900	0.	-1.000	0.00454	$-\infty$
0.40	2.50	-0.871	0.366	-0.987	0.166	0.66
0.60	1.67	-0.826	0.395	-0.931	0.370	0.90
0.80	1.25	-0.771	0.393	-0.848	0.438	0.89
1.0	1.00	-0.663	0.396	-0.762	0.420	0.90
1.2	0.833	-0.624	0.321	-0.682	0.371	0.88
1.4	0.714	-0.568	0.294	-0.613	0.318	0.92
1.6	0.625	-0.496	0.236	-0.555	0.270	0.87
1.8	0.556	-0.441	0.201	-0.505	0.230	0.86
2.0	0.500	-0.428	0.169	-0.462	0.197	0.88
2.2	0.455	-0.377	0.143	-0.426	0.169	0.84
2.4	0.417	-0.361	0.136	-0.394	0.147	0.92
2.6	0.385	-0.324	0.108	-0.367	0.128	0.84
2.8	0.357	-0.314	0.0971	-0.343	0.113	0.88
3.0	0.333	-0.296	0.0871	-0.322	0.0996	0.88
3.2	0.313	-0.278	0.0767	-0.303	0.0887	0.88
3.4	0.294	-0.253	0.0741	-0.286	0.0794	0.90
3.6	0.278	-0.258	0.0655	-0.271	0.0715	0.93
3.8	0.263	-0.227	0.0594	-0.257	0.0647	0.89
4.0	0.250	-0.216	0.0534	-0.245	0.0588	0.88

Table 3: Results of the 1D simulation for N = 100,  $N_{samples} = 1000$ .

		Numerical		Analytical		
T	$\beta$	$U_{/N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
0.20	5.00	-0.990	0.	-1.000	0.00454	$-\infty$
0.40	2.50	-0.990	0.00393	-0.987	0.166	-20
0.60	1.67	-0.989	0.0142	-0.931	0.370	-12
0.80	1.25	-0.889	0.0989	-0.848	0.438	-0.74
1.0	1.00	-0.821	0.180	-0.762	0.420	0.30
1.2	0.833	-0.790	0.146	-0.682	0.371	0.16
1.4	0.714	-0.613	0.290	-0.613	0.318	0.95

Table 3: continued

		Num	erical	Anal	Analytical	
T	$\beta$	U/N	$^{C}/_{\mathrm{N}}$	$U_{/N}$	$C_{/N}$	accuracy
1.6	0.625	-0.499	0.214	-0.555	0.270	0.81
1.8	0.556	-0.542	0.0760	-0.505	0.230	-0.049
2.0	0.500	-0.419	0.129	-0.462	0.197	0.69
2.2	0.455	-0.407	0.181	-0.426	0.169	0.94
2.4	0.417	-0.366	0.0847	-0.394	0.147	0.60
2.6	0.385	-0.384	0.0739	-0.367	0.128	0.61
2.8	0.357	-0.326	0.125	-0.343	0.113	0.92
3.0	0.333	-0.293	0.0890	-0.322	0.0996	0.89
3.2	0.313	-0.327	0.0840	-0.303	0.0887	0.93
3.4	0.294	-0.220	0.0893	-0.286	0.0794	0.79
3.6	0.278	-0.267	0.0392	-0.271	0.0715	0.58
3.8	0.263	-0.293	0.0608	-0.257	0.0647	0.91
4.0	0.250	-0.203	0.0425	-0.245	0.0588	0.71

Table 4: Results of the 1D simulation for N = 100,  $N_{samples} = 10000$ .

		Nume	erical	Analytical		
T	$\beta$	$U_{/N}$	$C_{/N}$	$U_{/N}$	$C_{/N}$	accuracy
0.20	5.00	-0.990	0.	-1.000	0.004 54	$-\infty$
0.40	2.50	-0.984	0.0547	-0.987	0.166	-0.021
0.60	1.67	-0.942	0.102	-0.931	0.370	-0.33
0.80	1.25	-0.835	0.595	-0.848	0.438	0.86
1.0	1.00	-0.785	0.379	-0.762	0.420	0.93
1.2	0.833	-0.683	0.296	-0.682	0.371	0.87
1.4	0.714	-0.583	0.302	-0.613	0.318	0.95
1.6	0.625	-0.549	0.253	-0.555	0.270	0.96
1.8	0.556	-0.497	0.193	-0.505	0.230	0.90
2.0	0.500	-0.444	0.179	-0.462	0.197	0.93
2.2	0.455	-0.423	0.138	-0.426	0.169	0.89
2.4	0.417	-0.396	0.127	-0.394	0.147	0.92
2.6	0.385	-0.359	0.128	-0.367	0.128	0.99
2.8	0.357	-0.343	0.110	-0.343	0.113	0.99
3.0	0.333	-0.319	0.136	-0.322	0.0996	0.86
3.2	0.313	-0.292	0.0805	-0.303	0.0887	0.93
3.4	0.294	-0.277	0.0802	-0.286	0.0794	0.98
3.6	0.278	-0.266	0.0744	-0.271	0.0715	0.97
3.8	0.263	-0.253	0.0735	-0.257	0.0647	0.93
4.0	0.250	-0.242	0.0643	-0.245	0.0588	0.95

Table 5: Results of the 1D simulation for  $N=1000,\,N_{samples}=1000.$ 

		Numerical		Analytical		
T	$\beta$	$U_{/N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
0.20	5.00	-0.999	0.	-1.000	0.004 54	$-\infty$
0.40	2.50	-0.999	0.	-0.987	0.166	$-\infty$
0.60	1.67	-0.999	0.	-0.931	0.370	$-\infty$
0.80	1.25	-0.983	0.102	-0.848	0.438	-0.72
1.0	1.00	-0.956	0.280	-0.762	0.420	0.65
1.2	0.833	-0.877	0.383	-0.682	0.371	0.87
1.4	0.714	-0.794	0.208	-0.613	0.318	0.62
1.6	0.625	-0.696	0.409	-0.555	0.270	0.73
1.8	0.556	-0.583	0.157	-0.505	0.230	0.70
2.0	0.500	-0.508	0.129	-0.462	0.197	0.69
2.2	0.455	-0.460	0.0419	-0.426	0.169	-0.56
2.4	0.417	-0.399	0.108	-0.394	0.147	0.82
2.6	0.385	-0.356	0.0345	-0.367	0.128	-0.37
2.8	0.357	-0.371	0.0357	-0.343	0.113	-0.11
3.0	0.333	-0.359	0.0296	-0.322	0.0996	-0.23
3.2	0.313	-0.351	0.0140	-0.303	0.0887	-1.7
3.4	0.294	-0.279	0.0241	-0.286	0.0794	-0.16
3.6	0.278	-0.268	0.0125	-0.271	0.0715	-1.4
3.8	0.263	-0.240	0.0112	-0.257	0.0647	-1.4
4.0	0.250	-0.230	0.0197	-0.245	0.0588	-0.025

Table 6: Results of the 1D simulation for N = 1000,  $N_{samples} = 10000$ .

		Numerical		Analytical		
T	$\beta$	$U_{\rm N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
0.20	5.00	-0.999	0.	-1.000	0.00454	$-\infty$
0.40	2.50	-0.999	0.	-0.987	0.166	$-\infty$
0.60	1.67	-0.988	0.0726	-0.931	0.370	-1.1
0.80	1.25	-0.937	0.479	-0.848	0.438	0.91
1.0	1.00	-0.805	0.928	-0.762	0.420	0.70
1.2	0.833	-0.685	0.193	-0.682	0.371	0.54
1.4	0.714	-0.629	0.173	-0.613	0.318	0.57
1.6	0.625	-0.520	0.406	-0.555	0.270	0.80
1.8	0.556	-0.511	0.243	-0.505	0.230	0.97
2.0	0.500	-0.476	0.190	-0.462	0.197	0.97
2.2	0.455	-0.430	0.187	-0.426	0.169	0.95
2.4	0.417	-0.389	0.181	-0.394	0.147	0.90
2.6	0.385	-0.368	0.0987	-0.367	0.128	0.85
2.8	0.357	-0.350	0.0720	-0.343	0.113	0.71

Table 6: continued

		Numerical		Analytical		
T	$\beta$	$U_{\rm N}$	$C_{/N}$	$U_{\rm N}$	$C_{/N}$	accuracy
3.0	0.333	-0.323	0.0659	-0.322	0.0996	0.74
3.2	0.313	-0.304	0.0913	-0.303	0.0887	0.98
3.4	0.294	-0.281	0.0695	-0.286	0.0794	0.92
3.6	0.278	-0.267	0.0773	-0.271	0.0715	0.96
3.8	0.263	-0.258	0.0544	-0.257	0.0647	0.90
4.0	0.250	-0.221	0.0854	-0.245	0.0588	0.79

# C. IMPLEMENTATION

# C.1. SIMULATION

**Listing 1:** ./../code/MMCIsing.m

Listing 2: ./../code/+neighbors/OneD2Connected.m

Listing 3: ./../code/+neighbors/TwoD4Connected.m

# C.2. STATISTICS

**Listing 4:** ./../code/computeAverageEnergy.m

Listing 5: ./../code/computeSpecificHeat.m

**Listing 6:** ./../code/computeAccuracy.m

Listing 7: ./../code/compute Average Magnetization.m

## C.3. EXPERIMENTS

**Listing 8:** ./../code/experiment\_1D.m

**Listing 9:** ./../code/experiment\_2D.m

# C.4. OUTPUT

Listing 10: .//code/tables_1D.m
Listing 11: .//code/+output/generateLaTeXTable.m
Listing 12: .//code/+output/plot.m
Listing 13: .//code/+output/private/filterExperiments.m
Listing 14: .//code/+output/private/collectData.m