One- and Two-Dimensional Ising Model

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September 6, 2016

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, $S_n = +1$, or down, $S_n =$ -1 [7]. The magnetization of a magnet is defined as its average spin:

$$\mathrm{M} = \left| \frac{1}{N} \sum_{i=1}^{N} S_i \right|,$$

where N is the number of spins. 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 one- and 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 $\{s_i\} = \{S_1, \ldots, S_N\}$ is

$$\mathcal{H} = -\mathcal{J} \sum_{\langle i,j \rangle} S_i S_j - \mathrm{h} \sum_i S_i. \tag{1}$$

Where $\langle i, j \rangle$ is a nearest neighbour pair, the nearest neighbour of S_i in the one dimensional model are S_{i-1} and 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 $\mathrm{h} = 0$, is considered. The energy E of a configuration of spins, $\{s_i\} = \{S_1, \ldots, S_N\}$, in this model is given by

$$E(\{s_i\}) = \sum_{n=1}^{N-1} S_n S_{n+1}.$$

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The probability of a configuration of spins $\{s_i\}$ at temperature T is given by

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

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

$$Z = \sum_{\{S_1,\dots,S_N\}} \exp\left[-E\beta\right]. \tag{2}$$

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 [4], the analytical solution of equation (2) is

$$Z = (2\cosh\beta)^N. \tag{3}$$

The average energy in the system can be expressed as a function of Z [5]

$$U = \frac{1}{Z} \cdot \sum_n E_n \cdot \exp\left[-\beta E_n\right].$$

Observing that

$$\frac{\partial Z}{\partial \beta} = \sum_n -E_n \exp\left[-\beta E_n\right],$$

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

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

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 [8], 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 $N \times N$ spins is computed as

$$\begin{aligned} E(\{s_n\}) = &-\sum_{i=1}^{N-1}\sum_{j=1}^{N} S_{i,j}S_{i+1,j} \\ &-\sum_{i=1}^{N}\sum_{j=1}^{N-1} S_{i,j}S_{i,j+1}. \end{aligned}$$

The two-dimensional Ising modle has been solved analytically by Onsager [6]. He showed that the average magnetization per spin on a infinite 2D lattice, i.e. $N = \infty$, is

$$\frac{\mathrm{M}}{N^2} = \begin{cases} \left(1-\sinh^{-4}(2\beta)\right)^2 & \text{if } T < T_c \\ 0 & \text{if } T > T_c \end{cases} \tag{4}$$

where

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

Given equation (2) 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. To be exact, a lattice with N spins has 2^N possible configurations, computing E according to equation (4) for one configuration takes $2N$ steps. This leads to $2N2^N$ computation steps [3]. Solving the problem with the Metropolis Monte Carlo method circumvents this complexity problem.

1.2. Metropolis Monte Carlo Methods

Consider random states, won't work, since ....

Metropolis MC in general

Importance sampling

The Metropolis solution

Use the general average stuff to show the next two functions.

How to compute average energy in the simulation

How to compute average magnetization in the simulation

What are we going to discuss in this paper?

2. Method

What are we going to discuss in this section?

beter structureren, splitsen in 1D en 2D?

how have we applied the MMC to the 1D and 2D ising model? Refer to appendix with actual implementation

3. Experiments

What are we going to discuss?

3.1. One-Dimensional Model

Wat gaan testen?

Average Energy

Define average energy for 1D

Report average energy for different values of T, N and NSAMPLES

Specific Heat

Define specific Heat for 1D

Report specific heat for different values of T, N and NSAMPLES

3.2. Two-Dimensional Model

Wat gaan we testen

Average Energy

Define average energy for 1D

Report average energy for different values of T, N and NSAMPLES

Specific Heat

Define specific Heat for 1D

Report specific heat for different values of T, N and NSAMPLES

Average Magnetization

Define magnetization

Report average magnetization for different values of T, N and NSAMPLES

4. 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, NSAMPLES

4.1. One-Dimensional Model

Present analytical solution i.e. prove whatever is one slide 28

Compare results with the analytical solution

4.2. Two-Dimensional Model

Compare Average magnetization with the exact result for the infinite system

5. Conclusion

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

Wat hebben we geleerd over de parameters.

References

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A. Mathematical Derivations

A.1. Average Energy[1]

$$
\begin{aligned}
U = \quad & -\frac{\partial \ln [Z]}{\partial \beta} \\
= & \{\textit{Definition of } Z \textit{ in equation } (3).\} \\
& -\frac{\partial \ln \left[(2\cosh\beta)^N\right]}{\partial \beta} \\
= & \left\{\textit{Chain rule: } \frac{\partial}{\partial \beta}\ln\left[2^N \cosh^N(\beta)\right] = \frac{\partial \ln [u]}{\partial u} 0,\ u = 2^n \cosh^n(\beta),\ \frac{\partial}{\partial u}\ln[u] = \frac{1}{u}\right\} \\
& -2^{-N}\cosh^{-N}(\beta)\left(\frac{\partial}{\partial \beta}\left(2^N \cosh^N(\beta)\right)\right) \\
= & \{\textit{Factor out constants.}\} \\
& -2^{-N}\frac{\partial}{\partial \beta}\left(\cosh^N(\beta)\right) 2^N \cosh^{-N}(\beta) \\
= & \{\textit{Simplify the expression.}\} \\
& -\cosh(\beta)^{-N}\left(\frac{\partial}{\partial \beta}\cosh^N(\beta)\right) \\
= & \left\{\textit{Chain rule: } \frac{\partial}{\partial \beta}\cosh^N(\beta) = \frac{\partial u^N}{\partial u} 0,\ u = \cosh(\beta),\ \frac{\partial}{\partial u}\left(u^N\right) = N \cdot u^{-1+N}\right\} \\
& -N\cosh(\beta)^{N-1}\frac{\partial}{\partial \beta}(\cosh(\beta))\cosh^{-N}(\beta) \\
= & \{\textit{Simplify the expression.}\} \\
& -N\left(\frac{\partial}{\partial \beta}\cosh(\beta)\right)\operatorname{sech}(\beta) \\
= & \{\textit{Derivative of } \cosh(\alpha) \textit{ is } \sinh(\alpha).\} \\
& -\sinh(\beta) N \operatorname{sech}(\beta) \\
= & \{\textit{Simplify the expression.}\} \\
& -N\tanh(\beta)
\end{aligned}
$$

A.2. Specific Heat

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

[1]The derivation has been computed with Wolfram Research, Inc. [9].

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