Studying second order phase transitions by using the Ising model in two dimentions and the metropolis algorithm

Project 4, FYS-3150

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Abstract

The aim of this project is to numerically solve ..... by using the .... algorithm.
the Ising model in two dimensions, without an external magnetic field
Title: Studying phase transitions (critical T) using the ising model (metropolis alg)?
compare teory, lars onsager

All source codes can be found at: `https://github.com/inakbk/Project_2`.

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bla bla theory and the programs

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3.1 The Ising model in two dimentions

The Ising model is a simple model for ferromagnetism in statistical physics. The model consists of magnetic spins that are allowed to interact with its neigbours. The magnetic dipole moments are allowed to have two values, 1 and -1.

In this project we will study the ising model i two dimentions wich allows the identification of phase transitions (define). We will also set the external magnetic field to zero troughout this paper.

The Ising model gives that the energy (for the whole system?) can be expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{1}$$

where the value of the spins are $s_k = \pm 1$ and N is the total number of spins. The variable J is a coupling constant expressing the strength of the interaction between neighboring spins.

The symbol $< kl >$ indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, viz $J > 0$ and use periodic boundary conditions.

(invlude matrix of spins and define variable L, N and M)

First we assume that there is only two spins in each dimention (x and y), we set $L = 2$. Then the closed form expression for the partition function is given by:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}$$

where M is the number of microstates or combinations of spins.

3.2 L=2 analytical values

$N = L \cdot L = 4$

There is $M = L^N = 2^N = 16$ microstates, or possible combinations and energies of the spin system. So to calculate the partition function we have to find the energies:

$$Z = e^{-\beta E_1} + ...e^{-\beta E_{16}}$$

The spin system can be visualized as 16 matrices on the form: $\begin{bmatrix} s(0,0) & s(0,1) \\ s(1,0) & s(1,1) \end{bmatrix}$ with corresponding energies.

Periodic boundaryconditions give that every spin has a neighbour. The neighbours of the spin $s(1,1)$ is $s(0,1)$ twice (above and below) and $s(1,0)$ twice (above and below). To find the energy we have to sum over the nearest neighbours for all the spins in the system. The product $s_l s_k$ of two neighbours should only be calculated once. This is solved if the index of s_l is fixed while s_k has one higher index in each direction at a time:

$$E = -J\Big(s(0,0)\cdot\big[s(1,0)+s(0,1)\big] + s(0,1)\cdot\big[s(1,1)+s(0,0)\big] + s(1,0)\cdot\big[s(0,0)+s(1,1)\big] + s(1,1)\cdot\big[s(0,1)+s(1,0)\big]\Big) \tag{2}$$

The 16 states with corresponding energies calculated with equation 2 is then:

$$\begin{array}{cccc}
E_1 = 0 & E_2 = 0 & E_3 = 0 & E_4 = 0 \\
\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} & \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} & \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} & \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix} \\
E_5 = 0 & E_6 = 0 & E_7 = 0 & E_8 = 0 \\
\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} & \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} & \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} & \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \\
E_9 = 0 & E_{10} = 0 & E_{11} = 0 & E_{12} = 0 \\
\begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} & \begin{bmatrix} -1 & -1 \\ 1 & -1 \end{bmatrix} & \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} & \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix} \\
E_{13} = 8J & E_{14} = 8J & E_{15} = -8J & E_{16} = -8J \\
\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} & \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} & \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} & \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}
\end{array}$$

We then see that there is only three possible values for the energies, $E \in \{-8J, 0, 8J\}$ with corresponding multiplicity $\{2, 12, 2\}$. The partition function can then be calculated:

$$\begin{aligned}
Z &= 2e^{-\beta(-8J)} + 12e^{-\beta\cdot 0} + 2e^{-\beta\cdot 8J} = 2(e^{\beta\cdot 8J} + e^{-\beta\cdot 8J}) + 12 \\
&= 4\cosh(8J\beta) + 12
\end{aligned}$$

using that $\cosh(x) = \frac{1}{2}(e^{-x} + e^{x})$.

Now that we have the partition function various expectation variables can be calculated. We start with the expectation value for the energy:

$$\begin{aligned}
\langle E\rangle &= \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i} = \frac{1}{Z}\big[2\cdot(-8J)e^{8J\beta} + 0 + 2\cdot 8Je^{-8J\beta}\big] = \frac{1}{Z}\big[-16Je^{8J\beta} + 16Je^{-8J\beta}\big] \\
&= -\frac{16J}{Z}\big[-e{-}8J\beta + e^{8J\beta}\big] = -\frac{32J}{Z}\sinh(8J\beta) = -\frac{8J\sinh(8J\beta)}{\cosh(8J\beta)+3}
\end{aligned}$$

using that $\sinh(x) = \frac{1}{2}(-e^{-x} + e^{x})$. We will now calculate the heat capacity

$$C_v = \frac{1}{k_b T}\sigma_E^2 = \frac{1}{k_b T}\big(\langle E^2\rangle - \langle E\rangle^2\big)$$

where

$$\begin{aligned}
\langle E^2\rangle &= \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} = \frac{1}{Z}\big[2\cdot(-8J)^2 e^{8J\beta} + 0 + 2\cdot(8J)^2 e^{-8J\beta}\big] = \frac{128J^2}{Z}\big[e^{8J\beta} + e^{-8J\beta}\big] \\
&= \frac{128J^2\cdot 2\cosh(8J\beta)}{4\cosh(8J\beta)+12} = \frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3}
\end{aligned}$$

so that

$$C_v = \frac{1}{k_bT}\left[\frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} - \left(-\frac{8J\sinh(8J\beta)}{\cosh(8J\beta)+3}\right)^2\right] = \frac{1}{k_bT}\left[\frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} - \frac{64J^2\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$
$$= \frac{64J^2}{k_bT}\left[\frac{\cosh(8J\beta)(\cosh(8J\beta)+3)-\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right] = \frac{64J^2}{k_bT}\left[\frac{\cosh^2(8J\beta)+3\cosh^2(8J\beta)-\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$
$$= \frac{64J^2\beta}{T}\left[\frac{1+3\cosh(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$

The magnetization is given by:

$$\mathcal{M} = \sum_{i=1}^{M} s$$

we quicly see that there are only 5 possible values for the magnetization, $\mathcal{M} \in \{-4, -2, 0, 2, 4\}$. The information on multiplicity for a given energy and magnetization is given in table 3.2.

# spins up	Multiplicy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

(abs val table? in 3.2)

abs Magnetization	Energy	Multiplicy
4	-8J	2
2	0	8
0	0	4
0	8J	2

The expectation value of the magetization is then:

$$\langle|\mathcal{M}|\rangle$$

absolute value???

We then want to calculate the suceptibility

$$\chi = \frac{1}{k_bT}\big(\langle\mathcal{M}^2\rangle - \langle\mathcal{M}\rangle^2\big)$$

where

$$\langle\mathcal{M}^2\rangle = \sum_{i=1}^{M}\mathcal{M}^2\frac{1}{Z}e^{-\beta E_i} = \frac{1}{Z}\big(2\cdot 4^2 e^{-\beta(-8J)} + 8\cdot 2^2 e^0 + 0 + 0\big) = \frac{32}{Z}\big(e^{8J\beta}+1\big)$$
$$= \frac{8\big(e^{8J\beta}+1\big)}{\cosh(8J\beta)+3}$$

so that

$$\chi = \frac{1}{k_bT}\big(\langle\mathcal{M}^2\rangle - \langle\mathcal{M}\rangle^2\big) =$$

wat? abs value or not?

3.3 Units, scaled unitless parameters

Introducing:

$$T' = T\frac{k_b}{J} \Rightarrow T = T'\frac{J}{k_b}$$
$$\beta = \frac{1}{k_b T} = \frac{1}{k_b \cdot T' \frac{J}{k_b}} = \frac{1}{T' J}$$

We then set $J = 1$ so that:

$$\beta = \frac{1}{T'}$$

where T' is the unitless parameter that will be used in the calculations (do with C_v' also and so on ??)

3.4 Coding dE and w efficiently

4 "Experiment"

4.1 Testing the implementation og model and algorithm

4.2 Studying the number of Monte Carlo cycles

4.3 Studying .... close to the critical temp

4.4 Calculations to find T_c

5 Results and output

6 Discussion and experiences

a) Assume we have only two spins in each dimension, that is $L = 2$. Find the closed form expression for the partition function and the corresponding expectations values for for E, $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions.

b) Write now a code for the Ising model which computes the mean energy E, mean magnetization $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions for $L = 2$ in the x and y directions. Compare your results with the expressions from a) for a temperature $T = 1.0$ (in units of kT/J).

   How many Monte Carlo cycles do you need in order to achieve a good agreeement?

c) We choose now a square lattice with $L = 20$ spins in the x and y directions.

   In [b) we did not study carefully how many Monte Carlo cycles were needed in order to reach the most likely state. Here we want to perform a study of the time (here it corresponds to the number of Monte Carlo cycles) one needs before one reaches an equilibrium situation and can start computing various expectations values. Our first attempt is a rough and plain graphical one, where we plot various expectations values as functions of the number of Monte Carlo cycles.

   Choose first a temperature of $T = 1.0$ (in units of kT/J) and study the mean energy and magnetisation (absolute value) as functions of the number of Monte Carlo cycles. Use both an ordered (all spins pointing in one direction) and a random spin orientation as starting configuration. How many Monte Carlo cycles do you need before you reach an equilibrium situation? Repeat this analysis for $T = 2.4$.

   Make also a plot of the total number of accepted configurations as function of the total number of Monte Carlo cycles. How does the number of accepted configurations behave as function of temperature T?

d) Compute thereafter the probability $P(E)$ for the previous system with $L = 20$ and the same temperatures. You compute this probability by simply counting the number of times a given energy appears in your computation. Start the computation after the steady state situation has been reached. Compare your results with the computed variance in energy σ^2_E and discuss the behavior you observe.

Near T_C we can characterize the behavior of many physical quantities by a power law behavior. As an example the mean magnetization is given by

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta}, \tag{3}$$

where $\beta = 1/8$ is a so-called critical exponent. A similar relation applies to the heat capacity

$$C_V(T) \sim |T_C - T|^{\alpha}, \tag{4}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{5}$$

with $\alpha = 0$ and $\gamma = 7/4$. Another important quantity is the correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{6}$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{7}$$

with a a constant and ν defined in Eq. (6). We set $T = T_C$ and obtain a mean magnetisation

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu}, \tag{8}$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \tag{9}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}. \tag{10}$$

e) We wish to study the behavior of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. Calculate the expectation values for $\langle E \rangle$ and $\langle |\mathcal{M}| \rangle$, the specific heat C_V and the susceptibility χ as functions of T for $L = 20$, $L = 40$, $L = 60$ and $L = 80$ for $T \in [2.0, 2.4]$ with a step in temperature $\Delta T = 0.05$ or smaller. Plot $\langle E \rangle$, $\langle 1\mathcal{M}1 \rangle$, C_V and χ as functions of T. Can you see an indication of a phase transition?

   Use the absolute value $\langle |\mathcal{M}| \rangle$ when you evaluate χ.

   You should parallelize the code using either OpenMP or MPI.

f) Use Eq. (7) and the exact result $\nu = 1$ in order to estimate T_C in the thermodynamic limit $L \rightarrow \infty$ using your simulations with $L = 20$, $L = 40$, $L = 60$ and $L = 80$ The exact result for the critical temperature (after Lars Onsager) is $kT_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ with $\nu = 1$.

Background literature

If you wish to read more about the Ising model and statistical physics here are two suggestions.

1. M. Plischke and B. Bergersen, Equilibrium Statistical Physics, Prentice-Hall, see chapters 5 and 6.

2. M. E. J. Newman and T. Barkema, Monte Carlo methods in statistical physics, Oxford, see chapters 3 and 4.