Numerical simulations of one-dimensional Ising model

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This project is devoted to study statistical properties of one dimensional Ising model.

I. INTRODUCTION

Ferromagnetism arises when a collection of atomic spins align such that their associated magnetic moments all point in the same direction, yielding a net magnetic moment which is macroscopic in size. The simplest theoretical description of ferromagnetism is called the Ising model. This model was invented by Wilhelm Lenz in 1920: it is named after Ernst Ising, a student of Lenz who chose the model as the subject of his doctoral dissertation in 1925. Although unpromising in its initial results, derived by Ising, the Ising model has turned out to be an exceptionally reach idea. The number of papers written on the subject is staggering; the number of papers which remain to written is conceivably even more staggering. Presently "Ising model" is one of the most frequent phrases in scientific literature.

A. Lattices

Our starting point for the Ising model is a *lattice*, which for us will be a finite set of regularly spaced points in a space of dimension $d = 1$,2, or 3. In dimension 1 we simply have a string of points on a line, which we can enumerate from 1 to N.

In our pictures, each lien segment between lattice sides is called a bond, and lattice sites are called *nearest neighbors* if there is a bond connecting them.

In general, except for lattice sites on the boundary of the lattice, each lattice site in a d-dimensional lattice has $2d$ nearest neighbors. Sometimes, the different between lattice sites on the boundary and those in the interior is inconvenient. Thus usually we work with the periodic boundary conditions when an extra bonds are introduced connecting lattice sides on opposite sides of the boundary. This amounts in wrapping a one dimensional lattice into a closed ring of spins.

To each lattice site we assign an independent variable σ_i, $i = 1, \ldots, N$. The variables σ_i describe magnetic moments of atoms and take only two values, $\sigma_i = \pm 1$, two possible states of the lattice site. An assignment of values $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ to each lattice site is called a *configuration* of the system. To find an average of an operator, we will need to sum over all possible configurations, 2^N.

B. Ising Hamiltonian

For the Ising model, the Hamiltonian is define under a sever assumption: it is assumed that only short-range, "nearest-neighbor" interactions and interactions of the lattice sites with an "external field" contribute to the energy

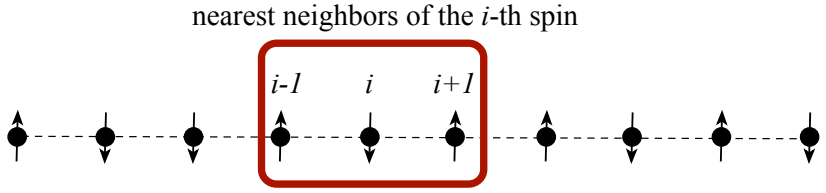

FIG. 1: Nearest neighbors for the one-dimensional Ising model with open boundary conditions.

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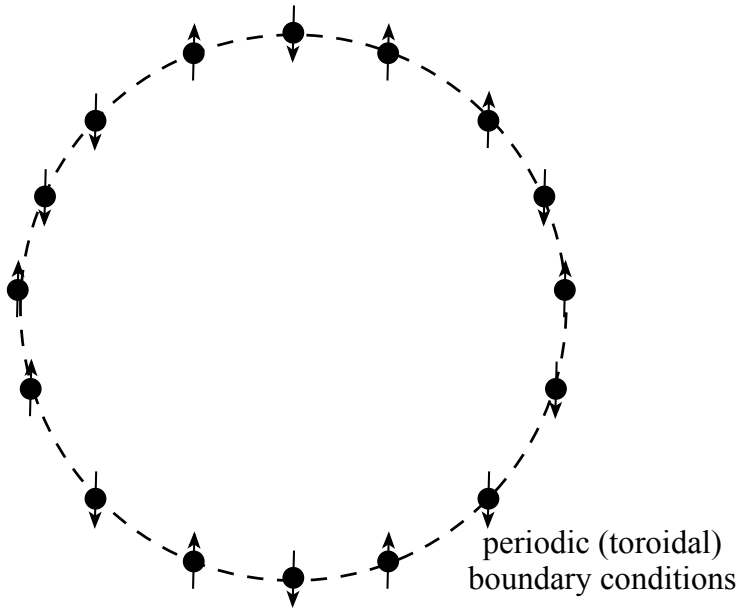

FIG. 2: Periodic boundary conditions for the one-dimensional Ising model.

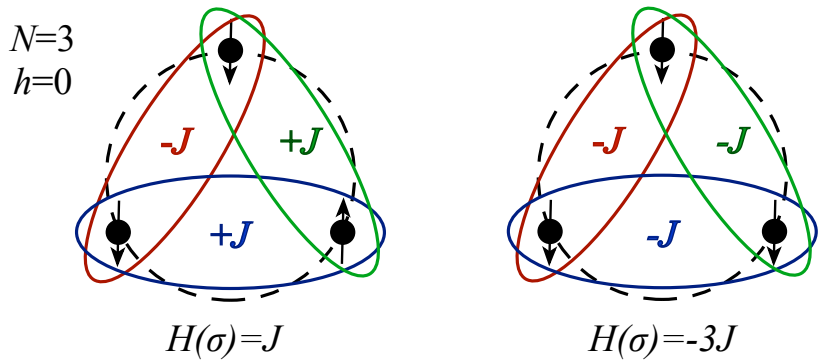

FIG. 3: Two configurations for the one-dimensional Ising model with the periodic boundary conditions and the number of spins $N = 3$, the external field is assumed to be zero. The total number of possible configurations is $2^N = 2^3 = 8$.

of the system. For each configuration $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ we have

$$H = H(\sigma) = -\sum_{\langle i,j \rangle} J\sigma_i\sigma_j - h\sum_i \sigma_i, \tag{1}$$

where h and J are parameters corresponding to the strength of nearest-neighbor interactions and interactions with the external field. The first sum is over all *pairs of nearest neighbors* in the lattice. h will tend to line up the the magnetic moments in the direction of the field.

C. Statistical mechanics of the Ising model

The partition function is given by

$$Z = Z(\beta, J, h, N) = \sum_\sigma e^{-\beta H(\sigma)}. \tag{2}$$

Where the sum is over all possible configurations of the system.

A simple example may help to clarify some of the notation. Let's take a very small one-dimensional lattice, consisting of $N = 3$ lattice sites with open boundary conditions. The hamiltonian is

$$H[(\sigma_1, \sigma_2, \sigma_3)] = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3) - h(\sigma_1 + \sigma_2 + \sigma_3). \tag{3}$$

To simplify matters further, we will consider $h = 0$. The partition function involves $2^3 = 8$ terms

$$\begin{aligned}
Z &= \exp(-\beta H[(1,1,1)]) + \exp(-\beta H[(1,1,-1)]) + \exp(-\beta H[(1,-1,1)]) && (4)\\
&+ \exp(-\beta H[(1,-1,-1)]) + \exp(-\beta H[(-1,1,1)]) + \exp(-\beta H[(-1,1,-1)]) && (5)\\
&+ \exp(-\beta H[(-1,-1,1)]) + \exp(-\beta H[(-1,-1,-1)]) && (6)\\
&= \exp(-\beta J(1+1)) + \exp(-\beta J(1-1)) + \exp(-\beta J(-1-1)) && (7)\\
&+ \exp(-\beta J(-1+1)) + \exp(-\beta J(-1+1)) + \exp(-\beta J(-1-1)) && (8)\\
&+ \exp(-\beta J(1-1)) + \exp(-\beta J(1+1)) && (9)\\
&= 2\exp(2\beta J) + 4 + 2\exp(-2\beta J) && (10)\\
&= 2^3 \cosh^2 \beta J. && (11)
\end{aligned}$$

Usually we redefine parameters of the model, so that β is measured in terms of inverse J and h in terms of J. This gives the "reduced" Hamiltonian

$$H_r = H_r(\sigma) = -\sum_{\langle i,j \rangle} \sigma_i\sigma_j - h\sum_i \sigma_i, \tag{12}$$

and thus the partition function depends only on dimensionless β, h and N. We will change the notation $H = H_r$.

II. THE METROPOLIS ALGORITHM

A. General problem

Suppose we want to calculate the exact partition function Z numerically. Need to do this for all β, but let's start with just one temperature. For a real system, want $\mathcal{O}(10^{23})$ spins, but let's start small and try to solve for a 1024-site lattice, i.e. $\mathcal{O}(10^3)$ spins. Number of configurations in the sum $= 2^{10^3} = 10^{300}$.

Suppose we had a gigantic parallel supercomputer, with ...10 million processors, CPU. Each processor could generate a configuration σ, calculate $H(\sigma)$ and the Boltzmann factor $\exp(-\beta H(\sigma))$ and add it to the sum over configurations in one nanosecond (less than the time for a single instruction for the fastest modern computer). And let's run this calculation for ...the age of the universe. This gives 10^7 CPU $\times 10^9$ configurations per second per CPU $\times 10^{14}$ sec/year $\times 10^{10}$ years $= 10^{40}$ configurations. Not even close to what we need, 10^{300} configurations.

In order to get sensible, accurate results when simulating statistical systems with a rapidly varying Boltzmann distribution, it is vital to use the idea of importance sampling in Monte Carlo integration.

Clearly the ideal situation would be to sample configurations with a probability given by their Boltzmann weight $p(\sigma)$, which gives a measure of their contribution to the sum total. Then the Monte Carlo average for any operator M on the lattice would just be:

$$\langle M \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} M(\sigma(i)), \tag{13}$$

where $\sigma(i)$ is a particular configuration and N_c is the number of configurations. It would work, except that the sampling probability $p(\sigma) = e^{-\beta H(\sigma)}/Z$ depends on the partition function Z, which is basically what we are trying to calculate in the first place!

Thus wee need to develop an algorithms to generate configurations distributed according to $p(\sigma)$ approximately.

B. Markov chain

Let us set up a so-called *Markov chain* of configurations σ_t by the introduction of a fictitious dynamics. The "time" t is computer time (marking the number of iterations of the procedure), NOT real time – our statistical system is considered to be in equilibrium, and thus time invariant.

Let $P(A,t)$ be the probability of being in configuration A at time t.
Let $W(A \to B)$ be the probability per unit time, or *transition probability*, of going from A to B. Then:

$$P(A,t+1) = P(A,t) + \sum_B \left[W(B \to A)P(B,t) - W(A \to B)P(A,t)\right]. \tag{14}$$

At large t, once the arbitrary initial configuration is "forgotten,"

$$\lim_{t\to\infty} P(A,t) \to p(A). \tag{15}$$

Clearly a sufficient (but not necessary) condition for an equilibrium (time independent) probability distribution is the so-called detailed balance condition

$$W(A \to B)P(A,t) = W(B \to A)P(B,t) \tag{16}$$

This method can be used for any probability distribution, but if we choose the Boltzmann distribution

$$\frac{W(A \to B)}{W(B \to A)} = \frac{p(B)}{p(A)} = \frac{\exp[-\beta H(B)]}{\exp[-\beta H(A)]} = \exp[-\beta \Delta H], \tag{17}$$

where $\Delta H = H(B) - H(A)$.

N.B. Equation (17) only involves quantities that we know (β) or can easily calculate (H). It does not involve Z!

This dynamic method of generating an arbitrary probability distribution was invented by Metropolis, Teller, and Rosenbluth in 1953 (supposedly at a Los Alamos dinner party). There are many possible choices of the W's which will satisfy detailed balance. The simplest one:

$$W(A \to B) = \begin{cases} \exp(-\beta \Delta H) & \text{if } \Delta H > 0 \\ 1 & \text{if } \Delta H \leq 0 \end{cases} \tag{18}$$

We will have a valid Monte Carlo algorithm if: We have a means of generating a new configuration B from a previous configuration A such that the transition probability satisfies detailed balance. The generation procedure is *ergodic*, i.e. every configuration can be reached from every other configuration in a finite number of iterations. The Metropolis algorithm satisfies the first criterion for all statistical systems. The second criterion is model-dependent, and not always true (e.g. at $T = 0$).

C. Algorithm realization for the 1d Ising model

The Metropolis algorithm for sampling the states of the one-dimensional Ising model in equilibrium with a heat bath at temperature β^{-1} is as follows:

1. Chose an initial configuration of N spins (lattice sites), e.g. all $\sigma_i = 1$.
2. Pick a spin at random and compute the trial change in energy, ΔH, that would occur if the spin were flipped.
3. If $\Delta H < 0$, accept the flip. If $r < \exp(-\beta \Delta H)$, where r is a uniform random number between 0 and 1, the change is also accepted; otherwise reject the flip and retain the original microstate. One Monte Carlo step per spin (mcs) is equivalent to N attempted spin flips.
4. Repeat steps 2 and 3 many times
5. Accumulate date for the various thermodynamic averages once the system reaches equilibrium.

D. Measurements

Suppose we generated configurations of the Ising model using a Monte Carlo algorithm, such as Metropolis. We want to numerically measure quantities of interest, such as:

$$E = \frac{1}{N_c}\sum_{\text{config}} E(\sigma) = \frac{1}{N_c}\sum_{\text{config}}\left(-\sum_{\langle i,j\rangle}\sigma_i\sigma_j\right), \tag{19}$$

$$\langle M\rangle = \frac{1}{N_c}\sum_{\text{config}}\left(\sum_i \sigma_i\right), \tag{20}$$

$$\Gamma(n) = \frac{1}{N_c}\sum_{\text{config}}\left(\sum_i \sigma_i\sigma_{i+n}\right) - M^2, \tag{21}$$

$$k_B T^2 C_V = \langle E(\sigma)^2\rangle - \langle E(\sigma)\rangle^2, \tag{22}$$

$$\chi = \langle M^2(\sigma)\rangle - \langle M(\sigma)\rangle^2. \tag{23}$$

where

$$\langle A(\sigma)\rangle = \frac{1}{N_c}\sum_{\text{config}} A(\sigma). \tag{24}$$

χ is the magnetic susceptibility and $\Gamma(n)$ is the correlations function, which is often used to extract the correlations length ξ (measured in lattice spacings) at $n \gg 1$ from

$$\Gamma(n) \propto \exp\left(-\frac{n}{\xi}\right). \tag{25}$$

III. PROBLEMS

1. (N) Choose $N = 512$ (or larger) and $h = 0$ and determine the energy and magnetization as a function of temperature, β^{-1}. Compare the computed results for the energy with the exact answer (known for the 1d Ising model) at zero magnetic field $h = 0$. Make sure that you run for a sufficient number of Monte Carlo steps per spin.
2. (N) Determine the heat capacity, C_V and the susceptibility, χ, as a function of temperature, β^{-1}. Discuss the qualitative temperature dependence of these quantities.
3. (A) Why is the mean value of the magnetization of little interest for the one-dimensional Ising model? Why does simulation usually give $M \neq 0$.
4. (N) Calculate the correlation length for $\beta = 1$ and $\beta = 2$.
5. (A) Why does the Metropolis algorithm become inefficient at low temperatures?

IV. APPENDIX A: IMPLEMENTATION OF PERIODIC BOUNDARY CONDITIONS

In one dimension, the periodic boundary conditions are implemented by noticing that the Hamiltonian can be written as

$$H = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - h\sum_{i=1}^{N}\sigma_i, \tag{26}$$

where $\sigma_{N+1} = \sigma_1$. We generally use periodic boundary conditions, where the lattice wraps around on itself to form a torus/a ring. This has been shown to give the smallest finite size effects.

But then we must be careful that in measuring the correlation function, we can only take measurements to $N/2$ for a lattice of size N, since a distance n is equivalent to a distance $n + N/2$ on a lattice that wraps around on itself.

V. APPENDIX B: THERMALIZATION

Before taking measurements, we must be sure that the Markov process has thermalized, or reached equilibrium, i.e. $P(A,t) = p(A)$ and the arbitrary initial configuration has been "forgotten." Usually approach to equilibrium is exponential $e^{t/\tau}$. The *autocorrelation* time can be very large. There are 3 main techniques for checking for thermalization:

- Binning: Check to see whether measurements are converging to a constant average value. Can do this by binning the data, i.e. splitting measurements up into a number of large contiguous segments (bins). Averages are taken over each bin, and data from initial deviant bins is discarded. *Binning can also be used to calculate errors.*
- Autocorrelations: Measure the autocorrelation time over the whole simulation, and then throw away data for at least the first 10τ sweeps. One *Monte Carlo sweep* is any N successful spin updates.
- Hot and cold starts: Start from hot (absolutely random) configuration and also a cold (ordered, all spins in one direction) configuration. When the two have converged to the same results, then usually the system is equilibrated[1].

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[1] Not the case for *a first order phase transition.*