Introduction to Computational Physics SS2019

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Exercise 11 from July 8, 2019
Return by noon of July 19, 2019 (this is the last exercise)

1 Ising Model – Introduction

The Ising model in two spatial dimensions can be used as a simple physical model for ferromagnetic behavior. We consider a quadratic mesh with n positions of atoms in each of the x and y directions, i.e. in total $N = n^2$ atoms. Suppose the atoms are fixed in a lattice and each has spin s_α, corresponding to an elementary magnetic moment. Note that all physical quantities are considered as numbers here, we skip for brevity dimensional scaling. Quantum mechanics prescribes that the spin can only be oriented in two directions with respect to some external axis, which we assume here to be the y-axis. We denote the two cases by $s_\alpha = 1$ (spin parallel to y-axis) or $s_\alpha = -1$ (anti-parallel). A configuration of our system is given by the set of spins s_α for $\alpha = 1, \ldots, N$. We denote such a configuration (sometimes also called a "spin state") with S_i. There is a very very large number of possible configurations, so i can be very large. The energy of a configuration S_i is

$$H(S_i) = -B \sum_\alpha s_\alpha - J \sum_{\langle \alpha\beta \rangle} s_\alpha s_\beta \tag{1.1}$$

where B denotes a possible external magnetic field. The summation index $\langle \alpha\beta \rangle$ denotes a summation over all direct neighbors of an atom (not diagonal, so we have only four neighbors in two dimensions). J is a spin-spin coupling constant; note that in the above double sum every pair of spins (m, n) occurs twice, once when (n) is a neighbour of $\alpha = m$ and another time, when (m) is a neighbour of $\alpha = n$. Our definition of J takes this already into account. Note that in some publications on the Ising model you find $J/2$ used instead, to make this clear.

$M = \sum_\alpha s_\alpha$ is a (dimensionless) measure of the total magnetic moment of the spin lattice, in the spin state S_i. Accordingly, $m = M/N$ is the magnetic moment per atom. In order to compare measurements of spin lattices with different size it is useful to normalize them per atom. We use here dimensionless units for the magnetic moment, for a spin lattice of size N the magnetic moment can just take any integer number from $-N$ to N, but note it is always $-1 \leq m \leq 1$. We use periodic boundary conditions, for example the neighbors of the leftmost column of spins to the left are identical to the rightmost column, and analogously for the uppermost and lowermost rows.

The expectation value of the magnetization $\langle m \rangle$ (total magnetic moment per atom) for a large number of spin states S_i, which are distributed according to a probability distribution

$w(S_i)$, is approximated by a Monte Carlo integral with weight $w(S_i)$

$$\langle m \rangle = \frac{1}{N} \sum_i w(S_i) M_i = \frac{1}{N N_S} \sum_i M_i = \frac{1}{N N_S} \sum_i \left(\sum_\alpha s_\alpha \right)_i \tag{1.2}$$

The first sum in the above equation runs over all allowed states of the system, which is an enormeous number. The second and third sums are running only over a number N_S of sweeps, which you have done in your experiment in order to obtain an ensemble of spin states. This number is only of the order of a few hundred. So we are substituting the weighted sum over all states by an average over selected few hundred states obtained by our Monte Carlo (Ising) model. The spin states obtained by the Ising model obey the canonical or Gibbs-Boltzmann distribution. The α sum for a spin state S_i is just the sum over the individual atomic spins. Free parameters are the spin coupling constant J, the external magnetic field B, and the temperature T (see below how it enters into the equations).

The probability distribution function of states of the canonical distribution is according to statistical thermodynamics

$$w(S_i) = \frac{\exp\left(-\beta H(S_i)\right)}{\mathcal{Z}} \; ; \; \mathcal{Z} = \sum_i \exp\left(-\beta H(S_i)\right) \tag{1.3}$$

with $\beta = 1/(kT)$ and the partition function (German: Zustandssumme) $\mathcal{Z}$. The partition function is generally too complicated to be computed directly, rather we use the Ising model to compute spin states which obey the probability distribution $w(S_i)$, without explicitly knowing $\mathcal{Z}$. The method is also called a Metropolis algorithm.

Consequently we can compute, as a second observable, the mean energy per atom of the system as

$$\langle e \rangle = \frac{1}{N} \sum_i w(S_i) H(S_i) = \frac{1}{N N_S} \sum_i H(S_i). \tag{1.4}$$

Our goal is to create by the Ising model a large number N_S of states, obeying $w(S_i)$. N_S cannot be nearly as large as the real number of possible states. In fact, it will be much much smaller. However, we can choose N_S large enough to get sufficiently accurate information about the average physical state of the system (such as the magnetization or the energy). The reason why this is possible lies in the fact that many of the possible states have a very low probability and contribute very little to the partition function. We focus on those states which have a higher probability and contribute significantly to the partition sum.

2 The Metropolis Algorithm for the Ising Model (hands-on tutorial)

In your numerical program for the Ising model you will do the following steps to reach the goal as described above:

1. First, generate an initially random configuration of spins. We introduce $b = \beta B$ and $j = \beta J$ and the Hamiltonian (energy) $h = \beta H$ as dimensionless numerical parameters. Test your algorithm for example by using $b = 0.0, 0.2$, $j = 0.25, 0.6$. Note that in this way the inverse temperature β does not occur explicitly in the equations. But we vary the temperature by varying the dimensionless parameter j, since the original parameter J has a constant physical value.

2. For every atom continue with the following procedure:

   - Choose randomly a new spin for the atom.
   - Is it the same as before, proceed to the next atom.
   - Is it different than the spin was before, compute the energy difference ΔE (use the Hamiltonian) between the old and new configuration. Is $\Delta E < 0$, the new configuration has a higher probability than the old one, and is accepted. Is $\Delta E > 0$ the new configuration will only be accepted with a probability $q = \exp(-\beta \Delta E) = \exp(-\Delta h)$. Note that q is the ratio of $w(S_i)$ for the new and old state. You check acceptance by comparing with a random number out of the interval 0,1.

3. Once you have done this procedure for all atoms, you have created a new spin state S_i (we also say you have done a "Sweep"). Compute its energy and magnetic moment, and save it. It will be used to compute the sums in (1.2) and (1.4) later.

4. After you have done a sufficient number of sweeps compute the expectation values for the magnetization and energy per atom. Whether the number of sweeps is sufficient can be estimated from the variation of the final result if adding more sweeps.

5. At the beginning you should do several sweeps (about a hundred), whose measurements are **not** used for the sums, in order to start with a sufficiently relaxed (thermalized) configuration that does not depend anymore from the initial state.

3 Ising Model – Numerical Solutions
(homework assignment – 20 points)

Use the Metropolis method to obtain numerical solutions for the two dimensional Ising model and compare to the analytic approach.

a) First consider the Ising model in the "mean-field" approximation,

$$m_{\mathrm{mf}} = \tanh(b + 4jm_{\mathrm{mf}}) \quad ; b_{\mathrm{mf}} = b + 4jm_{\mathrm{mf}} = b + 4j\left(\frac{e^{b_{\mathrm{mf}}} - e^{-b_{\mathrm{mf}}}}{e^{b_{\mathrm{mf}}} + e^{-b_{\mathrm{mf}}}}\right) .$$

Use $j = 0.6$ and compute the magnetization m as a function of the magnetic field b. Plot the result (hysteresis). (6 points)

b) Now turn to the numerical solution using the Metropolis algorithm introduced above. Compute the mean energy $\langle e \rangle$ and magnetisation $\langle m \rangle$ per atom as a function of the magnetic field. Use a grid length of about 30, i.e. 900 atoms. Test the program for $j = 0$; in this case the mean field approximation provides the exact result. Solve the Ising model afterwards for at least two other values of j (recommended values $j \leq 0.4$ and $j \geq 0.5$). Plot the mean energy and magnetisation per atom as a function of the external magnetic field. Describe your observations. The high j value corresponds to a small temperature, we will get ordered (ferromagnetic) states, for the low j value (high temperature) we expect less order. In fact there is a critical value for j, at which the transition between ferromagnetic and non-ferromagnetic state occurs. Can you find it? (14 points)