Tutorial Introduction to Computational Physics SS2011

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Ising Model

Introduction

The Ising model is a simple description of ferromagnetism in two spatial dimensions. 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; 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 $\alpha = 1, \ldots, n^2$. We denote such a configuration (sometimes also called a "spin state") with S or S_i; note that there is a very very large number of possible configurations, so i can be very large. The energy of a configuration S is

$$H(S) = -B \sum_\alpha s_\alpha - J \sum_{\langle \alpha\beta \rangle} s_\alpha s_\beta \tag{0.1}$$

where B denotes a possible external magnetic field. The summation index $\langle \alpha\beta \rangle$ denotes a summation over all direct neighbours of an atom (not diagonal, so we just have only four neighbours in two dimensions). J is a spin-spin coupling constant. Note that $M = \sum_\alpha s_\alpha$ is a (dimensionless) measure of the total magnetic moment of our spin lattice, in the spin state S. $m = M/N$ is the magnetic moment per atom (to compare measurements of spin lattices with different size it is useful to normalise 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 neighbours 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 (average of spin states with weight according to $w(S_i)$)

$$\langle m \rangle = \frac{1}{N} \sum_i w(S_i) M_i = \frac{1}{N N_S} \sum_i M_i = \frac{1}{N N_S} \sum_i \left(\sum_\alpha s_\alpha \right)_i \tag{0.2}$$

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 as above is (for one spin state) the sum over the atom's spins. Free parameters are here 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

$$w(S_i) = \frac{\exp\left(-\beta H(S_i)\right)}{\mathcal{Z}} \; ; \; \mathcal{Z} = \sum_i \exp\left(-\beta H(S_i)\right) \tag{0.3}$$

with $\beta = 1/T$ 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

$$\langle e \rangle = \frac{1}{N} \sum_i w(S_i) H(S_i) = \frac{1}{N N_S} \sum_i H(S_i). \tag{0.4}$$

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 (actually it will be much much smaller); however, we can choose N_S large enough that we get sufficiently accurate informations about the average physical state of the system reliably (magnetisation, 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.

Programming the Metropolis algorithm

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

1. generate an initially random configuration of spins. $b = \beta B$ and $j = \beta J$ and the Hamiltonian (energy) $h = \beta H$ are used as dimensionless numerical parameters. Test your algorithm for example 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 proceed 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 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 $w(S)$ 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 (0.2) and (0.4) later.

4. After you have done a sufficient number of sweeps compute the expectation values for the magnetisation 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 (thermalised) configuration, which does not depend anymore from the initial state.

Ising Model Home Work

- 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 magnetisation m as a function of the magnetic field b (hysteresis plot) (6 points).

- Ising model with the Metropolis algorithm (MRRTT algorithm). 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 ither 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 exists a critical value for j, at which the transition between ferromagnetic and non-ferromagnetic state occurs. (14 points)