Homework 6; due Tuesday, November 20

PY 502, Computational Physics (Fall 2012)

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MONTE CARLO SIMULATION OF A DILUTED ISING MODEL

In class we discussed the Ising model, where spins $\sigma_i = \pm 1$ occupy the sites of a square lattice. The spins are coupled with a pair interaction $-J\sigma_i\sigma_j$. Here you will consider a modified 2D square-lattice Ising model in which the spin variable can also take the value 0; this value corresponds to an empty site. The model is illustrated in Fig. 1. It can describe, e.g., two different species of atoms or molecules ($\sigma_i = \pm 1$) partially covering a surface. We here take the interaction energy to be

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma \in \{-1, 0, 1\}, \tag{1}$$

where $\langle i, j \rangle$ is a pair of nearest-neighbor lattice sites (each pair counted only once) on an $L \times L$ lattice with periodic boundary conditions.

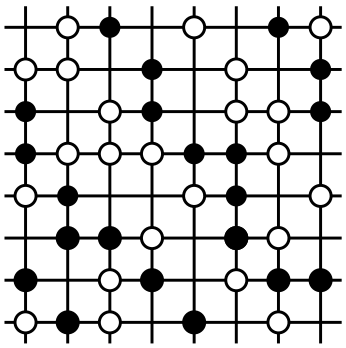

Figure 1: A configuration of the diluted 2D Ising model. Open and solid circles correspond to $\sigma = \pm 1$ (spin "up" and "down"), and an empty site indicates that no spin is present (a "hole").

Note that spins $\sigma_i = 0$ do not contribute to the energy. We set $J = 1$ (i.e., ferromagnetic interaction for spin pairs with $|\sigma_i| = |\sigma_j| = 1$). We can consider the system as a *diluted* magnet where the sites with $\sigma_i = 0$ sites are *empty* and those with $\sigma_i = \pm 1$ are *occupied* by magnetic moments (Ising spins). It is then useful to introduce the *occupation number* n_i as

$$n_i = |\sigma_i|, \quad (\text{occupation number} = 0, 1), \tag{2}$$

so that $n_i = 0$ and $n_i = 1$ correspond to empty and occupied sites, respectively.

We now use V to denote the number of sites (equal to the volume if the lattice spacing equals unity); $V = L^2$. The number of occupied sites,

$$N = \sum_{i=1}^{V} n_i, \tag{3}$$

is not fixed because the configuration space includes all 3^V combinations of $\sigma_i = 0, \pm 1$; think of the ± 1 spins as being allowed to move around on the lattice, and also spins can flow in an out of the system (leading to fluctuations in N). This corresponds to a grand-canonical ensemble (here at zero chemical potential). The density expectation value $n = \langle N \rangle / V$ will therefore depend on the temperature.

You will use Monte Carlo simulations to study the phase transition to a magnetized state occurring in this diluted Ising model. As before, by symmetry the expectation value $\langle M \rangle$ of the magnetization,

$$M = \sum_{i=1}^{V} \sigma_i, \tag{4}$$

is zero for a finite system, and hence we instead study $m = \langle |M| \rangle / V$ and $\langle M^2 \rangle$, from which we can also obtain the susceptibility (normalized per site);

$$\chi = \frac{1}{T} \frac{1}{V} (\langle M^2 \rangle - \langle |M| \rangle^2). \tag{5}$$

The susceptibility is the linear response of the magnetization to a magnetic field h (derived by adding a term $-hM$ to the energy and taking the derivative $\chi = dm/dh$ at $h = 0$). In an analogous way, the compressibility κ is the response of the particle density to a chemical potential μ (derived by adding a term $-\mu N$ to the energy and taking the derivative $\kappa = dn/d\mu$ at $\mu = 0$) and is given by the fluctuation of the particle number;

$$\kappa = \frac{1}{T} \frac{1}{V} (\langle N^2 \rangle - \langle N \rangle^2). \tag{6}$$

We use e to denote the energy per volume; $e = \langle E \rangle / V$. The specific heat is given by the energy fluctuation:

$$c = \frac{1}{T^2} \frac{1}{V} (\langle E^2 \rangle - \langle E \rangle^2). \tag{7}$$

We will also be interested in the Binder ratio,

$$Q = \frac{\langle M^2 \rangle}{\langle |M| \rangle^2}, \tag{8}$$

as a way to locate the phase transition through the crossing points for Q versus T for different L.

Programming task

Write a Metropolis Monte Carlo program to simulate the diluted Ising model on periodic $L \times L$ lattices (arbitrary L, periodic boundary conditions). The program should be able to do simulations for several equally spaced temperatures in a single run, starting from the highest one. The input data should be read from a file "read.in" in the following format:

```
nt, tmax, dt
bins, steps
```

where `nt` is the number of temperatures, `tmax` the highest temperature, `dt` the temperature spacing, `bins` the number of bins to do for each temperature, and `steps` the number of Monte Carlo steps per bin (with a step defined as $V = L^2$ random updates).

You can the simple (but good) 64-bit random-number generator function `ran()` available on the course web site (also used in `ising2d.f90` and in the test programs `rantest.f90`, where you can see how to properly declare and initialize it). It needs a single integer seed, which should be read from a file "seed.in".

The program should measure the quantities discussed above; $\langle E \rangle$, $\langle E^2 \rangle$, $\langle M \rangle$, $\langle M^2 \rangle$, $\langle N \rangle$, and $\langle N^2 \rangle$. The bin data should be processed (calculating averages and statistical errors) by another program, which also should calculate the quantities c, χ, κ, and Q, according to the expressions given above. The final processed output should be written to files "e.dat", "m.dat", "p.dat", and "q.dat" in the following way (one line for each temperature):

`e.dat`: $T,\ e,\ \sigma_e,\ c,\ \sigma_c$
`m.dat`: $T,\ m,\ \sigma_m,\ \chi,\ \sigma_\chi$
`n.dat`: $T,\ n,\ \sigma_n,\ \kappa,\ \sigma_\kappa$
`q.dat`: $T,\ Q,\ \sigma_Q$

Programming hints and tests

When you attempt to "flip" (update) a spin, you now have two new states to choose from (e.g., if $\sigma_i = -1$ you can change it either to 0 or 1). The new state should be selected at random. As always, the Metropolis acceptance probability is

$$P_{\text{accept}} = \mathrm{e}^{-\Delta E/T}, \tag{9}$$

where $\Delta E = E_{\text{new}} - E_{\text{old}}$.

There are several obvious checks you can do on your program in the high and low temperature limits: As $T \to \infty$ all configurations become equally probable and hence $n \to 2/3$. The lowest-energy states are those that have all $\sigma_i = 1$ or all $\sigma_i = -1$ (and hence there should be a phase transition for some $T_c > 0$). Therefore, $e \to -2$, $n \to 1$, and $m \to 1$ as $T \to 0$. Getting these limits right does not necessarily mean that your program is correct, however. You are also given the following information to help in testing your program: The critical temperature T_c (and associated susceptibility and specific heat peaks for all system sizes $L \geq 4$) is between 1 and 2 (in units where $J = 1$). If you want to be completely confident that your program is correct, you can also carry out exact calculations for some very small lattices, i.e., generating all 3^V configurations and averaging measurements done on them with the Boltzmann factor $\mathrm{e}^{-E/T}$ (the 3×3 system can be done easily and 4×4 without too much effort). These results can then be compared with Monte Carlo results for the same V.

Calculations and reporting of results

Do simulations for system sizes $L = 4$, 8, 16, etc., going to as large lattice size as you can within your available computer resources (or whatever size you need to extract the wanted information).

Graph the energy e, the magnetization m, the density n, the specific heat c, the susceptibility χ, and the compressibility κ versus temperature for the different system sizes (one graph for each quantity, different sizes in the same graphs). Use a linear or logarithmic scale for the y-axis, whichever gives a clearer view of the behavior of each quantity.

Locate the critical temperature T_c at which there is a phase transition into a ferromagnetic state, using the Binder ratio crossings, the specific heat, and the susceptibility.

Based on the calculated density curve $n(T)$ and knowing that the critical temperature for the standard 2D Ising model is $T_c^{\rm Ising}/J \approx 2.27$, how could you estimate T_c for the diluted model? Hint: Assume that the holes are randomly distributed and consider an effective interaction $J_{\rm eff}/J$ arising from the probability of two nearest-neighbor sites both being occupied. What is this estimate and how does it compare with the actual T_c that you found?

Investigate the divergence of the peak height of the susceptibility, i.e., graph $\ln(\chi)$ versus $\ln(L)$ to approximately find the exponent γ from the slope (i.e., if the form $\chi \sim L^\gamma$ holds). You can use the line-fitting program available on the course web-site, or any other software of your choice, to extract the slope γ. How does the exponent compare with that of the standard 2D Ising model (discussed in the lecture notes)? What kind of divergence, if any, do you find for the specific heat? Again, compare with the standard 2D Ising model. You should not expect the results to be as good (smooth curves) as those discussed in class for the standard 2D sing model, because those results were generated with a much more efficient cluster algorithm. You are only asked to obtain some rough estimates of the exponents here, based on what is feasible with a single-spin method and your available computer resources.

Unlike the magnetization (in the limit of infinite system size), the density n is non-zero both above and below T_c. The phase transition concerns the magnetic properties of the model, but nevertheless there can be some signs of the transition also in the density and the compressibility. What kind of behavior do you find in the compressibility at the phase transition? Is there a divergence or some other non-analytic behavior?

Note that the physics server `buphy0` is available for your long calculations for course-work (same log-in credentials as for `buphy`, on which you should not do any long calculations).