Computational Science 2

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Seminar Exercises

Exercise 6 (2.6.2020):

The 2D Ising model

from ***An Introduction to Computer Simulation Methods***,
Chapter 15, Problem 15.12,13,15-17

Because we will consider the Ising model for different values of the linear dimension L, it will be convenient to convert quantities to intensive quantities such as the mean energy per spin $\langle E \rangle$, the specific heat (per spin) C, the mean magnetization per spin $\langle M \rangle$, and the susceptibility per spin χ. For simplicity, we use the same notation as for the corresponding extensive quantities.

a) Write a target class that uses class `Ising` and plots the magnetization M and energy E as a function of the number of Monte Carlo cycles *mcc*. Your program also should display $\langle M \rangle$, $\langle E \rangle$, C, χ, and the acceptance probability when the simulation is stopped. Choose $L = 32$ and the heat bath temperature $T = 2$. Estimate the time needed to equilibrate the system given that all the spins are initially up.

b) Visually determine if the spin configurations are "ordered" or "disordered" at $T = 2$ after equilibrium has been established.

c) Repeat part (a) with the initial direction of each spin chosen at random. Make sure you explicitly compute the initial E and M in `initialize`. Does the equilibration time increase or decrease?

d) Repeat parts (a)-(c) for $T = 2.5$.

e) Choose $L = 4$ and the direction of each spin initially at random, and equilibrate the system at $T = 3$. Look at the time series of M and E after every *mcc* and estimate how often M changes sign. Does E change sign when M changes sign? How often does M change sign for $L = 8$, $L = 16$, and $L = 32$? Although the direction of the spins is initially chosen at random, it is likely that the number of up spins will not exactly cancel the number of down spins. Is that statement consistent with your observations? If the net number of spins is up, how long does the net M remain positive for a given value of L?

f) The calculation of χ is more complicated because the sign of M can change during the simulation for smaller values of L. Compare your results for χ using

$$\chi = \frac{1}{kT}(\langle M^2 \rangle - \langle M \rangle^2), \tag{1}$$

and using the above equation with M replaced by $|M|$. Which way of computing χ gives more accurate results?

g) The exact value of E/N for the Ising model on a square lattice with $L = 16$ and $T = T_c = 2/\ln(1+\sqrt{2})$ is given by $E/N = -1.45306$. It allows us to determine the actual error in this case. Compute E by averaging E after each mcc for at least 10^6 mcc. Compare your actual error to the estimated error $\sigma_m = \sigma/\sqrt{n}$ with $\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2$ and discuss their relative values.

h) Choose $L = 4$ and consider T in the range $1.5 \leq T \leq 3.5$ in steps of $\Delta T = 0.2$. Choose the initial condition at $T = 3.5$ such that the orientation of the spins is chosen at random. Because all the spins might overturn and the magnetization change sign during the course of your observation, estimate the mean value of $|M|$ in addition to that of M. Use at least 1000 mcc and estimate the number of equilibrium configurations needed to obtain M and E to 5% accuracy. Plot E, M, $|M|$, C, and χ as a function of T and describe their qualitative behavior. Do you see any evidence of a phase transition? Repeat the calculations for $L = 8$ and $L = 16$. Is the evidence of a phase transition more obvious?

i) Use the relation $T_c(L) - T_c(L = \infty) \sim L^{-1/\nu}$ together with the exact result $\nu = 1$ to estimate the value of T_c for an infinite square lattice. Because it is difficult to obtain a precise value for T_c with small lattices, we will use the exact result $kT_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$ for the infinite lattice in the remaining parts of this problem.

j) Determine $|M|$, C, and χ at $T = T_c$ for $L = 4, 8, 16$, and 32. Compute χ with $|M|$ instead of M. Use as many mcc as possible. Plot the logarithm of $|M|$ and χ versus L and use the scaling relations to determine the critical exponents β and γ. Use the exact result $\nu = 1$. Do your log-log plots yield reasonably straight lines? Compare your estimates with the exact values.

k) Make a log-log plot of C versus L. If your data for C is sufficiently accurate, you will find that the plot is not a straight line but shows curvature. The reason is that the exponent α equals zero for the two-dimensional Ising model, and hence $C \sim 0.4995 \ln L$. Is your data for C consistent?