Physics 642 Final Project: Monte Carlo Methods

Due Date: 12/08/2021 1:00 PM

Instructions

You should hand in a report answering all parts of question 1 as well as working code with instructions on how to run it (either by uploading your code to canvas along with the report, or including a link to a public repository). You may use any programming language you are comfortable with.

Some general hints and strategies:

- A basic introduction to Monte Carlo methods with working code can be found at: `https://github.com/agdelma/IntroMonteCarlo`.
- Make sure you test and debug your code for a *small* system size, say $L = 4$. This will enable you to get rapid feedback without run time delays.
- Separate the generation of data from plotting. You should write data files for each estimator (e.g. $\langle E \rangle, \langle M \rangle$) as a function of Monte Carlo step. This will allow you to perform statistical analyses and plot without having to rerun your simulation.
- For part (d), Goldenfeld has nice discussion of finite size scaling.

1. Classical Monte Carlo for the 2D Ising Model **[50 points]**

Consider the 2D Ising model,

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

where $\langle i, j \rangle$ indicates that the sum is over only nearest neighbor spins and $\sigma_i = \pm 1$. We will work in units where $J = +1$ (ferromagnetic), $k_{\mathrm{B}} = 1$ and employ periodic boundary conditions for a lattice with $N = L \times L$ spins.

Write a Monte Carlo simulation for the 2D square-lattice Ising model using Metropolis "importance" sampling. Construct the simulation state to consist of the Ising spin variables at each lattice site. Starting from a random initial state, choose trial states based on their Boltzmann weight as follows:

i. A trial configuration is made by randomly flipping one spin.

ii. The energy difference (ΔE) between the trial state and the old state is is calculated.

iii. If $\Delta E < 0$, the trial state is energetically favored and therefore accepted. If $\Delta E > 0$, a random number $0 \leq r \leq 1$ is generated, and the trial state is accepted only if $\exp(-\beta \Delta E) > r$.

The thermodynamic energy $\langle E \rangle$ and total magnetization $\langle M \rangle$ can be estimated from the average over samples:

$$\langle E \rangle = \frac{1}{N_{\mathrm{MC}}} \sum_{n=1}^{N_{\mathrm{MC}}} E_n$$

$$\langle M \rangle = \frac{1}{N_{\mathrm{MC}}} \sum_{n=1}^{N_{\mathrm{MC}}} M_n$$

where the sum is over all $N_{\rm MC}$ iterations of the above Monte Carlo algorithm and E_n, M_n are the energy and magnetization of the $n^{\rm th}$ configuration $\left\{\sigma_1^{(n)}, \ldots, \sigma_N^{(n)}\right\}$:

$$E_n = -\sum_{\langle i,j \rangle} \sigma_i^{(n)} \sigma_j^{(n)}$$

$$M_n = \sum_{i=1}^{N} \sigma_i^{(n)} \, .$$

(a) For a $L = 16$ lattice (256 sites) at $\beta = 1/T = 1$ and 3, plot the average energy (per spin) $\langle E \rangle / N$ as a function of Monte Carlo iteration (or "time") step n. There should be an initial warm-up period where the energy changes rapidly, before fluctuating around an equilibrium. Data during this initial warm-up period should not be included in the thermodynamic averages calculated below.

(b) Produce a plot of the average energy per spin $\langle E \rangle / N$ and order parameter per spin $\langle M \rangle / N = \langle \sigma_i \rangle$ versus temperature making sure to average over at *least* 10^5 Monte Carlo steps per temperature. Do the limits $T \to 0$ and $T \to \infty$ match your theoretical expectations? Include the exact results from the Onsager solution (included in the Bonus question below, setting $J = k_{\rm B} = 1$) on your plot and discuss the agreement.

(c) Using your previously derived relation: $C_V = [\langle E^2 \rangle - \langle E \rangle^2]/T^2$, plot C_V versus T and obtain a rough estimate of the critical temperature, T_c. Again compare with the exact result included below in the Bonus question.

(d) Using your previously derived expression for the magnetic susceptibility, $\chi = [\langle M^2 \rangle - \langle M \rangle^2]/T$, plot χ versus T for a $L = 12, 16, 20$ and 24 size system. By using the exact Ising critical temperature $T_c = 2/\ln\left(1+\sqrt{2}\right)$, collapse the data as best as possible onto one curve, by plotting $\chi L^{-\gamma/\nu}$ versus $tL^{1/\nu}$. In this way, extract the critical exponents γ and ν. How do they compare to the exact values? Discuss your various sources of error?

BONUS: Exact Solution of the 2D Ising Model

In his remarkable solution[1] of the 2D Ising model, Onsager generalized the transfer matrix method you previously used in Assignment 1 to the case of a 2D rectangular lattice in zero magnetic field. This calculation was the first exact solution of a model displaying a phase transition. Onsager's original solution to the problem is quite complex, and many more straightforward methods have since been invented, including the mapping to a 1D fermionic problem[2]. Research this latter method and present a complete and detailed (with all intermediate steps) solution to the model on the square lattice. Define $K = \beta J$.

(a) Show that the internal energy per spin is given by:

$$e(T) = -J \coth 2K \left[1 + \frac{2}{\pi}(2\tanh^2 2K - 1) K_1(q)\right]$$

where

$$q(K) = \frac{2\sinh 2K}{\cosh^2 2K}$$

and

$$K_1(q) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - q^2 \sin^2 \phi}}$$

is the complete elliptic integral of the first kind.

(b) Taking another derivative, find the specific heat per spin:

$$k_{\rm B}^{-1} c_V(T) = \frac{4}{\pi} (K \coth 2K)^2 \left\{K_1(q) - E_1(q) - (1 - \tanh^2 2K)\left[\frac{\pi}{2} + (2\tanh^2 2K - 1) K_1(q)\right]\right\}$$

where

$$E_1(q) = \int_0^{\pi/2} d\phi \sqrt{1 - q^2 \sin^2 \phi}$$

is the complete elliptic integral of the second kind.

(c) Find the magnetization per spin:

$$m(T) = \left[1 - \frac{(1 - \tanh^2 K)^4}{16 \tanh^4 K}\right]^{1/8}$$

for $T < T_c$ and show that this gives the order parameter critical exponent $\beta = 1/8$ near T_c. To do this, you will need to use the previously quoted result that $k_B T_c/J = 2/\ln\left(1 + \sqrt{2}\right)$ which is equivalent to $\sinh 2J/k_B T_c = 1$. Yang[3] found an alternate method for computing m that does not use the fermion mapping if you are interested.

[1] L. Onsager, Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition, Phys. Rev. **65**, 117 (1944).

[2] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Two-Dimensional Ising Model as a Soluble Problem of Many Fermions, Rev. Mod. Phys. **36**, 856 (1964).

[3] C. N. Yang, The Spontaneous Magnetization of a Two-Dimensional Ising Model, Phys. Rev. **85**, 808 (1952).