Computational Physics II — Project 4

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In total, **100 + 20 pts** can be achieved by solving the problems below (see annotation).

Metropolis algorithm for the Ising model

Both the Metropolis algorithm and the Ising model have a huge number of applications, ranging from condensed matter physics to computational social science. The Ising model is one of the simplest models that experiences a continuous phase transition. Consider a 2D spin-$\frac{1}{2}$ Ising model

$$\mathcal{H} \equiv -J \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

on a square lattice, consisting of $N \equiv L \times L$ sites. In Eq. 1, assume that $J > 0$, that is, the energy of a state is lowered when spins align. The symbol $\langle i,j \rangle$ denotes any of the $2N$ nearest neighbor bonds. Further assume periodic boundary conditions, mimicking complete translational symmetry.

Expectation values of an observable A for the Hamiltonian $\mathcal{H}$ are given by

$$\langle A \rangle = \frac{1}{Z} \sum_{s_1=\pm1, s_2=\pm1, \dots, s_N=\pm1} A(s_1, s_2, \dots, s_N) e^{-\mathcal{H}/k_B T} . \tag{2}$$

1. (**20 pts**) Without running any simulations, can you "guess" and describe the ground state, i.e., the state for $T = 0$? What is the g.s. energy $\langle \mathcal{H} \rangle$ and its magnetization per site $|\langle m \rangle| = \frac{1}{N}|\langle \sum_{i=1}^{N} s_i \rangle|$? What is the energy difference between the g.s. and the first excited state? For the opposite limit, $T \to \infty$, what do you expect for the correlations $\langle s_i s_j \rangle$ between neighboring spins (*Hint*: consider the limiting value of the probability weights $\lim_{T \to \infty} e^{-\mathcal{H}/k_B T}$)? What are $\langle \mathcal{H} \rangle$ and $\langle m \rangle$ in the $T' \to \infty$ limit?

2. Write a computer program where you define the sites $i \in \{1, \dots, N\}$ and their spins $s_i \in \{-1, +1\}$. Start with a small number of sites $L \times L$, say $L = 20$. For convenience, work in dimensionless units where $\mathcal{H}' = \mathcal{H}/J$ and $T' = Tk_B/J$.[1] (**10 pts**)

3. *Parameter and initial condition.* (**10 pts**) Define T' as a parameter and initially set $T' = .1$. As an initial condition, set each spin to one of the two options at random. Define a function that computes the total system energy of a given (single) N-particle spin configuration, i.e.,

$$E' \equiv -\sum_{\langle ij \rangle} s_i s_j , \tag{3}$$

here, s_i and s_j are the configurations of the spins at site i and j for this given configuration.

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[1]In practical terms this amounts to setting $k_B = J = 1$ and working with $T' = \mathcal{O}(1)$.

4. *Site update.* (**10 pts**) Define a function that "flips" a randomly-selected spin i, $s_i \rightarrow -s_i$, as well as the exponential $r \equiv \exp{(-\Delta E'/T')}$, where $\Delta E' \equiv E'_j - E'_i$ is the energy difference between two states j and i. Define the acceptance procedure for a transition $w_{i \rightarrow j}$ using the Metropolis algorithm,

$$w_{i \rightarrow j} = \begin{cases} 1 \text{ , if } r > 1 \\ r \text{ , if } r < 1 \,. \end{cases} \tag{4}$$

5. *System update.* Code a function that produces N attempted site updates, hence, each site is considered once on average (due to randomness, some sites will not be updated but others multiple times). Carry out one system update (**10 pts**).

6. *Reaching convergence.* Call the system update a sufficiently large number of times n_0 (maybe start with $n_0 \approx 100$ but be ready to increase n_0 if needed). After each system update compute E' (see Eq. 3) and, analogously, the magnetization per site $|m| = |\frac{1}{N} \sum_{i=1}^{N} s_i|$ for the given configuration. Plot a "timeseries" of these values for $n \in [0, n_0]$. By inspecting the plot, estimate the value $n_{min} < n_0$, so that the numerical expectation values are not strongly affected by the transient behavior for $n > n_{min}$. (Note that you may need to make adequate adjustments to n_0 in this process, to be able to detect convergence.) By averaging all values for E' and $|m|$ for $n > n_{min}$ determine a more accurate numerical estimate of averages of E' and $|m|$, thus approximating the actual expectation values (**20 pts**).

7. By adjusting T', analogously obtain numerical expectation values for E' and $|m|$ at $T' \in \{0.1, 0.5, 1.0, 1.5, 2.0, 2.25, 2.5, 3.0, 10.0\}$ and plot them as function of T' by averaging the data obtained from samples for $n > n_{min}$. At this stage, note that the rate of convergence to equilibrium will depend on the value of T', hence, again, n_{min} may need to be adjusted. To visualize, for each T' plot a 2D "map" of the spin configuration for the final stage at n_0 (**10 pts**).

8. For the 2D Ising model an exact result exists, where $\langle m \rangle^8 = 1 - [\sinh(2/T')]^{-4}$ for $0 < T' < T'_c$, for $T'_c = 2/\ln(1 + \sqrt{2})$ and $\langle m \rangle = 0$ for $T' > T'_c$ (Onsager's solution [1]). Discuss in how far your numerical results agree with this solution (**10 pts**).

9. (**10 pts extra credit**). Using different random number seeds, repeat the simulation several times for each observable and temperature to obtain a distribution of results for that data point. Use the distribution to quantify the sampling error and plot the error bars.

10. (**10 pts extra credit**). Repeat for a larger system size L and make notes of your findings for n_{min} and discuss (qualitatively) how n_{min} and the error bars depend on system size.

General remarks for all Projects. You will have to (i) analyze the problem, (ii) select an algorithm (if not specified), (iii) write a Python program, (iv) run the program, (v) visualize the data numerical data, and (vi) extract an answer to the physics question from the data. Which checks did you perform to validate the code? State the results you got for these tests. For each project you will submit a short report describing the physics problem, your way of attacking it, and the results you obtained. Provide the documented Python code in such a form that we can run the code. A Jupyter Notebook including the code and report is fine but not necessary.

References

[1] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117, 1944.