Responsible TA: Samuel Bird, sabird@phys.ethz.ch
Exercise class in HCI J7.

Exercise 1. ***Monte Carlo simulation of the classical 2D Ising model with local updates***

Write a Monte Carlo simulation of the classical Ising model on an $L \times L$ square lattice. The classical Ising Model is described by the Hamiltonian

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

where $\langle i, j \rangle$ denotes nearest neighbour indices and the Ising spins can take values $s_i \in \{-1, +1\}$. We assume periodic boundary conditions and work in the canonical ensemble. This model is known to have a ferromagnetic (ordered) phase for temperatures $T < T_c$ and a disordered phase for $T > T_c$. In the limit $L \to \infty$, the phase transition occurs at the critical temperature $T_c \approx 2.269 J/k_B$.

Use the Metropolis algorithm, which generates a Markov chain of states by repeating the following steps:

- Choose a site i;
- Calculate $\Delta E = 2 J s_i h_i$;
- Generate the next configuration in the Markov chain by flipping spin s_i with probability $\min\left(1, e^{-\frac{\Delta E}{k_B T}}\right)$.

Here $h_i = \sum_{\langle i,j \rangle} s_j$ is the neighbour field of spin s_i (make sure you understand why the formula for ΔE is correct). It is useful to choose $J = 1$ and $k_B = 1$. In order to decouple from the system size you should count updates in units of sweeps, where one sweep corresponds to $N = L \cdot L$ single spin updates.

To measure the time average of a quantity Q we use the ergodic hypothesis and obtain

$$\langle Q \rangle_{\text{time}} \approx \overline{Q} := \frac{1}{M} \sum_{k=0}^{M-1} Q_k, \tag{2}$$

where M is the length of the sampled Markov chain and Q_k is the value of Q in the k-th state of the chain. The value of $\overline{Q}$ is only meaningful with an error estimate. Naively, we would calculate the statistical error Δ_Q via the variance,

$$\Delta_Q = \sqrt{\frac{\text{var}(Q)}{M}}, \tag{3}$$

$$\text{var}(Q) \approx \frac{M}{M-1} \overline{Q^2} - \overline{Q}^2 \tag{4}$$

$$= \frac{1}{M-1} \sum_{k=1}^{M} (Q - Q_k)^2 \tag{5}$$

However, this estimate is only good if the samples are uncorrelated. For correlated samples (as often present in Markov chains) this underestimates the true errors. Instead, one needs to generate uncorrelated samples, for example using the binning method.

Measure the absolute value of the magnetization $\langle |m| \rangle = \frac{1}{N} |\sum_i s_i|$ for different temperatures $T \in [0, 5]$. Plot the behavior with error bars. Analyze autocorrelation effects and take care of them using the binning method.

Hint. : Whenever you move to a new temperature, you should first equilibrate the system. This is done by performing update steps without measuring. The number of equilibration steps should roughly be of the same order of magnitude as the number of measurement steps.

Exercise 2. ***Monte Carlo simulation of the classical 2D Ising model with cluster updates***

As you should have realized in the previous exercise, local updates become inefficient at low temperatures and close to the phase transition. This behaviour can be improved by using cluster updates instead.

Implement the Wolff algorithm, which samples states by repeating the steps:

- Choose a site i randomly to seed the cluster;
- Add all neighbouring sites that are in the same state as s_i to the cluster with probability $1 - e^{-2\beta J}$;
- Repeat this for all sites on the boundaries of the cluster until all bonds of the cluster have been checked exactly once;
- Flip all spins in the cluster.

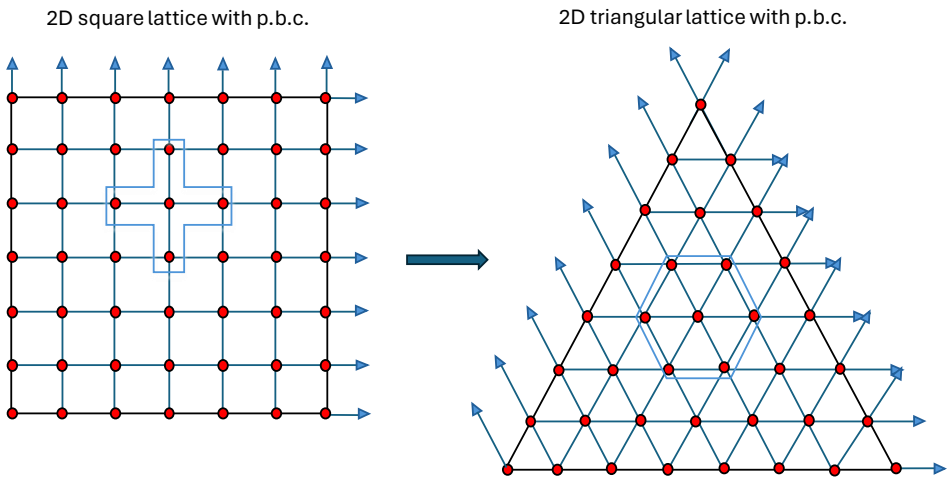
Reproduce the data found in exercise 1 by performing normal measurements (no improved estimators). Compare the autocorrelation effects that are observed in the two algorithms.

Exercise 3. ***2D Ising model on triangular lattice with LLM***

The Ising model serves as a fundamental concept in statistical mechanics, allowing us to study phase transitions and critical phenomena in various physical systems. While the square lattice Ising model provides valuable insights, extending our simulation to a triangular lattice introduces new complexities and behaviors to explore.
The triangular Ising model is described by the same Hamiltonian as the square lattice Ising model (see eq. 1), with slight modifications to account for the lattice geometry. Instead of considering nearest neighbors along orthogonal directions, we now consider nearest neighbors along the edges of equilateral triangles. This adjustment alters the interaction patterns between spins and introduces intriguing properties not present in the square lattice counterpart. The comparison between square and triangular lattice geometry is shown in the figure below.

In this exercise, you will build upon your existing implementation of the 2D square lattice Ising model and adapt it to simulate the Ising model on a triangular lattice. Instead of starting from scratch, you can exploit the capabilities of the large language model (ChatGPT) to guide you through the necessary modifications.

Procedure:



- Identify the necessary changes: use ChatGPT to perform the modifications required to transition from a square lattice to a triangular lattice. This includes adjustments to the lattice geometry, neighbor interactions, and boundary conditions.
- Apply the changes provided by ChatGPT to make your code suitable for simulating the triangular lattice. While ChatGPT can provide valuable guidance, it's important to remember that it may occasionally make mistakes or not optimal solutions. Therefore, it's essential to review and verify the implementation according to your understanding of the problem.
- Run the simulations at different temperatures in the range $T \in [0, 5]$ and study the behavior of the magnetization as a function of the temperature. In the limit $L \to \infty$, the phase transition for this model occurs at $T_c \sim 3.641 J/k_B$.

Addendum: Binning Analysis

The binning analysis starts from a series of (correlated) measurements $Q_i^{(0)} = Q_i$. One then iteratively generates new arrays of data that contain less correlations, by grouping adjacent data entries into pairs and replacing them by their averages. Recursively, the ℓth level array is thus given by

$$Q_i^{(\ell)} = \frac{1}{2}\left(Q_{2i}^{(\ell-1)} + Q_{2i+1}^{(\ell-1)}\right), \tag{6}$$

note that the array length M_ℓ is halved in each binning step. For the binned arrays, the estimate from equation 3 is

$$\Delta_Q^{(\ell)} = \sqrt{\frac{1}{M_\ell(M_\ell - 1)} \sum_{i=0}^{M_\ell - 1} \left(\overline{Q^{(\ell)}} - Q_i^{(\ell)}\right)^2}, \tag{7}$$

and increases with the binning level. These errors converge to the true value when the bin size (the number of datapoints collected in one bin) exceeds the integrated autocorrelation time τ_Q (the time over which correlations survive). The integrated autocorrelation time can be calculated

via

$$\tau_Q = \frac{1}{2}\left[\left(\frac{\Delta Q}{\Delta_Q^{(0)}}\right)^2 - 1\right], \tag{8}$$

where Δ_Q is the true value of the statistical error, i.e., $\lim_{\ell\to\infty} \Delta_Q^{(\ell)}$.

For your analysis in the exercises, you should perform roughly the following steps:

- Plot the behavior of $\Delta_Q^{(\ell)}$ as a function of ℓ. The curve should grow and saturate.
- Find a binning level ℓ for which $\Delta_Q^{(\ell)}$ saturates.
- If you cannot find such a level, you need more data, so longer simulation times.

  Hint. : At the phase transition, the autocorrelation time diverges.
- Use equation 6 to calculate error bars.
- What trend do you observe when looking at the binning level required as a function of temperature?
- Optional: Plot an estimate of the integrated autocorrelation time τ_Q as a function of temperature.

At the very least, you should check at several temperatures that your error estimates make sense. In order to facilitate the binning analysis, it is useful to choose the number of samples as a power of 2.

More information can be found in the paper https://arxiv.org/pdf/0906.0943.pdf, especially in sections IV-C and IV-D.