Project #2

Hunting vortices

Deadline: 14.12.2026, 12:00

Introduction

You are probably familiar with the Ising model and the symmetry-breaking transition it undergoes at low temperatures in 2D. In this project you will simulate a close relative, the *XY model*, which shows a rather unusual phase transition driven by tiny whirls, the *vortices*. You will then train a classifier on snapshots of this model on a square lattice and find out whether it can locate the phase transition.

The XY model

The XY model lives on the same $L \times L$ grid with periodic boundary conditions as the Ising model. The difference: instead of pointing up or down, each spin is described by a 2D vector which can point in any direction in the xy plane and is parameterized by an angle $\theta_i \in [0, 2\pi)$. Here we consider the ferromagnetic XY model, where neighboring spins prefer to point in the same direction, which is expressed by the energy

$$E(\theta) = -\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j),$$

where $\theta = (\theta_1, \ldots, \theta_{L^2})$ is the configuration of the entire grid and the sum runs over all pairs of nearest neighbors (left, right, up, down).

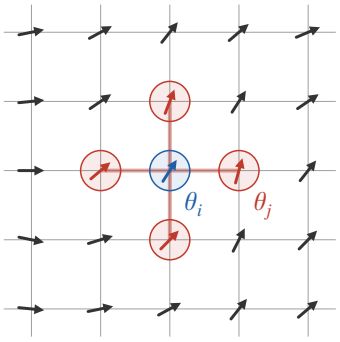


Illustration of the XY-model
Shown is a small patch of the grid. Each arrow is a spin with angle θ_i. The four nearest neighbors j (red) of the spin i (blue) are connected to it by bonds, and each bond contributes $-\cos(\theta_i - \theta_j)$ to the energy.

We will simulate this model using a classical Monte Carlo algorithm where, as for the Ising model, a configuration occurs at temperature T with probability

$$p(\theta) \propto e^{-E(\theta)/T}.$$

The magnetization per spin is now a vector, $m = \frac{1}{L^2}\,|\sum_i(\cos\theta_i, \sin\theta_i)|$. Since we have defined this model in 2D, the continuous rotation symmetry changes the physics: in the thermodynamic limit, the magnetization is always vanishing at any finite temperature. At low T the spins are nearly aligned, but their direction slowly drifts over large distances, so that $m \to 0$ for $L \to \infty$ at any $T > 0$. On a finite grid, however, m stays large at low T.

The actual phase transition is driven by *vortices*. On the grid, the vorticity of a plaquette (a square of four neighboring spins with angles $\theta_1, \ldots, \theta_4$ in counterclockwise order) is

$$v = \sum_{n=1}^{4} s\,(\theta_{n+1} - \theta_n)\,, \qquad s(x) = x - 2\pi\,\mathrm{round}\Big(\frac{x}{2\pi}\Big)\,, \qquad \theta_5 \equiv \theta_1,$$

which is the discretized line integral $\oint \nabla\theta \cdot \mathrm{d}\boldsymbol{\ell}$ around the plaquette. Without a vortex the turns cancel, $v = 0$. At a vortex (antivortex) they add up to one full turn, $v = +2\pi$ (-2π). Thus $v = 2\pi w$ with $w \in \{0, +1, -1\}$. Vortices are created by thermal fluctuations. Below the critical temperature

$$T_{\mathrm{KT}} \approx 0.893,$$

they only occur as tightly bound vortex–antivortex pairs, which hardly disturb the alignment of distant spins. Above T_{KT}, the pairs break apart and free vortices destroy any order. This is the Kosterlitz–Thouless transition, awarded the Nobel Prize in Physics 2016.

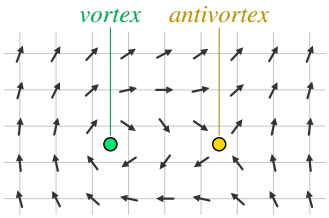
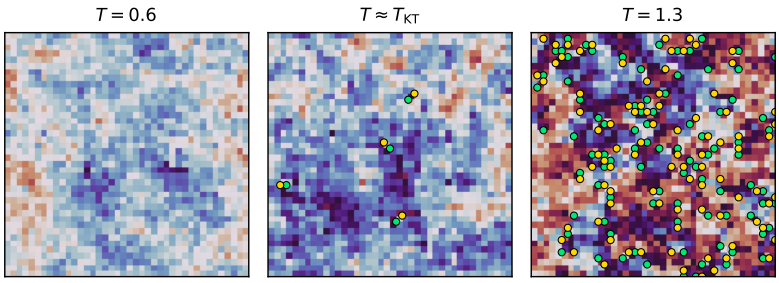


Illustration of a vortex pair
Around the vortex (green dot) the arrows turn counterclockwise by one full turn, around the antivortex (yellow dot) clockwise. Seen from far away, the two cancel and the arrows are nearly aligned.



Snapshots of the XY model A 40×40 grid at temperatures below, at and above T_{KT}. The color encodes the angle θ_i.

Simulating the XY model

We generate typical configurations with the *Metropolis algorithm*:

1. Pick a spin i and propose a new angle $\theta_i' = \theta_i + \delta$, with δ drawn uniformly from $[-\Delta, \Delta]$.
2. Compute the energy change $\Delta E = -\sum_j [\cos(\theta_i' - \theta_j) - \cos(\theta_i - \theta_j)]$, where j runs over the four neighbors of i.
3. Accept the new angle with probability $\min\left(1, e^{-\Delta E/T}\right)$.

Repeating this L^2 times is one *sweep*. Choose the step width Δ such that roughly half of the proposals are accepted (small Δ at low T). Since a spin only interacts with its four neighbors, all spins on the black fields of a checkerboard can be updated at once, then all spins on the white fields. Many independent grids, e.g. at different temperatures, can be simulated at once by stacking them into a single array. Keep in mind:

- Discard the first sweeps (equilibration) and leave some sweeps between recorded configurations, since consecutive configurations are correlated.
- At low T, vortex pairs from a random initial configuration take very long to annihilate. Start from aligned spins instead, each grid with a random common direction.

Task 1 – Simulation

Implement the Metropolis algorithm for the XY model in NumPy, vectorized over the spins of the grid (no Python loops over spins). Show that your simulation works, e.g. via snapshots, the average energy, m and the vortex density as functions of T for a few grid sizes L.

Machine learning the phase transition

Generate a dataset of configurations at many temperatures around T_{KT}, say $0.3 \leq T \leq 1.5$, and label each configuration by its phase, $T < T_{\mathrm{KT}}$ or $T > T_{\mathrm{KT}}$. The classifier is only given the configuration, never its temperature. Note that the angles 0 and 2π describe the same spin, so think about how to encode the configuration.

To estimate T_{KT}, apply the trained classifier to a test set and plot the fraction of configurations classified as "high T" against T. The temperature where it crosses $1/2$ is your estimate.

Task 2 – Classifier

Train a support vector machine (SVM) to classify spin configurations by phase. Compare different kernels (linear, polynomial, RBF). Estimate T_{KT} and compare to the value above. Why does a linear kernel fail? Compare the decision function to m and E, what does the SVM learn? Try using the vortex configuration w instead of the spins as input.

Task 3 – Neural network

As a second step, train a neural network in PyTorch on the same data to classify the phase. Compare to the SVM: accuracy, estimate of T_{KT}, and training effort. Try both the spins and the vortex configuration w as input. Beach *et al.*[1] found that networks trained on the raw spins learn the magnetization instead of the vortices. Can you reproduce this? Compare different grid sizes L. Try a fully connected and a convolutional neural network.

Task 4 – Presentation

Present your results and methodology in a short presentation in the tutorial after the deadline. The format is up to you. Everybody in your group must be able to answer questions about the project.

[1] M. J. S. Beach, A. Golubeva, R. G. Melko, *Machine learning vortices at the Kosterlitz-Thouless transition*, Phys. Rev. B **97**, 045207 (2018).