Predicting the Critical Temperature of the Ising Model

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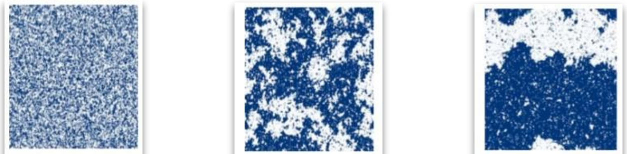
Introduction

The **Ising model**:

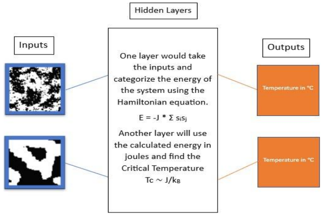
- **Purpose**: A mathematical model of particle ferromagnetism represented in 1-D or 2-D.
- **Nearest neighbor**: adjacent particles interact (isotropic), particles align/anti-align based on the sign of "J" to go toward lower energy. (Hamiltonian: $\mathbf{E = -J * \Sigma\, s_i s_j}$)
- **Critical Temperature**: a second order phase transition occurs (symmetry w/in model, scale invariant patterns), high T = disorder, **paramagnetic** vs. low T = order, **ferromagnetic**)

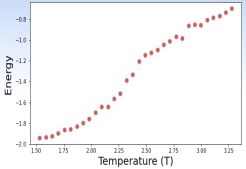


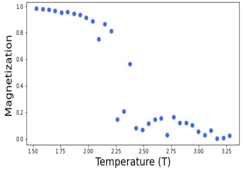
high temperature | "critical" temperature | low temperature

Methods/Procedures

Given an initial state, a machine learning model trained with a dataset of spin configurations can predict the critical temperature of the given state with high accuracy.

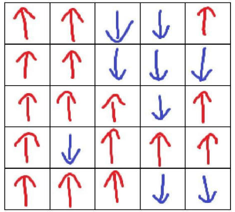


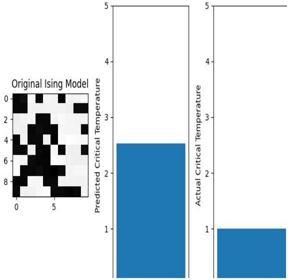




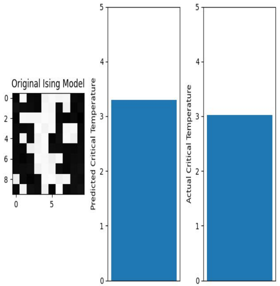
Pick a random site and calculate its energy;
Pick a random number $x \in (0,1)$;
for all sites **do**
  if $\Delta E < 0$ OR $x < e^{-\frac{\Delta E}{k_B T}}$ **then**
    Flip spin;
  else
    Do not flip spin
  end
end

$$p_{\text{flip}} = e^{-\frac{\Delta E}{k_B T}}$$





Results with less trained data



Results with more trained data

Goals

- Understand the mechanisms behind the Ising Model and the physical meaning the model has to real life structures (magnet, alloy, lattice gas)
- Connect ideas, like critical temp, presented in the Monte Carlo simulation to an application of machine learning (pattern recogn.)
- Compute Thermodynamic Quantities of Magnetic Particles to study and interpret (visual data)
- Combine Monte Carlo and machine learning to increase accuracy and fine tune model (apply to quantum computing at later stages)

Acknowledgements

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References

Jar, J. (2019). The Ising Model. The Ising model. https://stanford.edu/~jeffjar/statmech/intro4.html

The Code

ML-Specific | Ising Model