Machine-learning Assisted Monte-Carlo Simulations of an Ising Model

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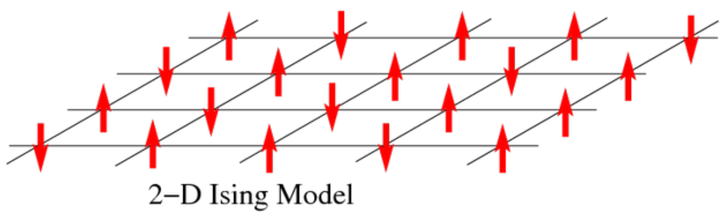
Ising Model Simulation Algorithms

An Ising Model represents a ferromagnet in which its magnetic dipoles are placed in a lattice, spun either up or down.



2–D Ising Model

The energy from the interactions between spins $S_i = \pm 1$ is:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - K \sum_{ijkl \in \square} S_i S_j S_k S_l$$

We want to create a simulation that correctly represents the thermal state of the collection of the dipoles as a function of thermal disorder and the energy between interacting spins.

A Monte Carlo step is the simulation of every dipole in the lattice as having a potential flip in its spin.

The **Metropolis Algorithm** selects a dipole at random and its spin configuration C_i updates with a probability given by:

$$p^{accept}(C_i \rightarrow C_j) = \min[\frac{e^{-E(C_j)/T}}{e^{-E(C_i)/T}}, 1]$$

The **Cluster Algorithm** selects a group of bonded dipoles at updates the spin configuration with a probability of 1/2. Neighboring dipoles are bonded with a probability given by:

$$\begin{aligned} P(\tau_b = 1) &= 1 - e^{2|J|/T}, && \text{if } \sigma_{i(b)} = \sigma_{j(b)} \\ P(\tau_b = 1) &= 0, && \text{if } \sigma_{i(b)} \neq \sigma_{j(b)} \end{aligned}$$

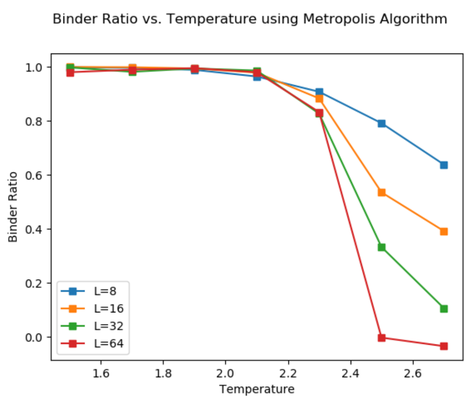
Ising Model Observables

The Binder cumulant is defined such that the intersection point of the system sizes will approach the critical temperature, where the system undergoes a phase from a paramagnetic to a ferromagnetic state.

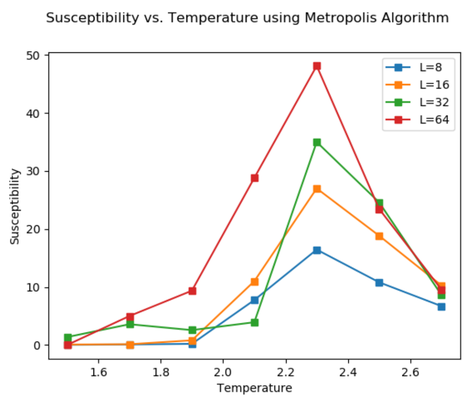
$$U_2 = \frac{3}{2}(1 - \frac{1}{3}\frac{\langle m^4 \rangle}{\langle m^2 \rangle^2})$$

The susceptibility describes the change in magnetization in response to an external field. It exhbiits a peak at the critcal temperature, whichgrows with the sytem size.

$$\chi = \frac{1}{N}\frac{1}{T}(\langle M^2 \rangle - \langle M \rangle^2)$$



$$\langle x \rangle = \frac{1}{n}\sum_{i=1}^{n} x_i$$

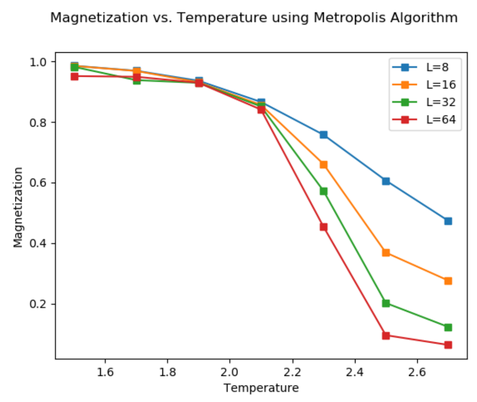


Magnetization and Autocorrelation

The magnetization of an Ising Model is defined as the average value of the dipole spins. It is zero in the paramegnetic phase and (its absolute value is) non-zero in the ferromagnetic phase.

Our data is collected over 10,000 Monte Carlo steps. The coefficients for nearest neighbor weights for the data below are J=1, K=0.

$$m = \frac{1}{N}\sum_{i=1}^{N} \sigma_i$$

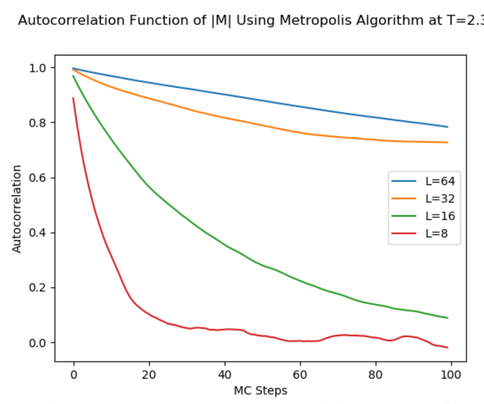


At the critical temperature, the autocorrelation time diverges algebraically with system size and hence one must simulate an increasingly longer time to generate statisically independent ensembles. We aim to design a machine learning algorithm that decreases the amount of Monte Carlo steps required for the model to thermalize.

The autocorrelation function measures the statisical significance of the difference in magnetization between Monte Carlo steps.

$$A_Q(\tau) = \frac{\langle Q_k Q_{k+\tau} \rangle - \langle Q_k \rangle^2}{\langle Q_k^2 \rangle - \langle Q_k \rangle^2}$$

$$\Theta_{\text{int}} = \frac{1}{2} + \sum_{\tau=1}^{\infty} A_Q(\tau)$$

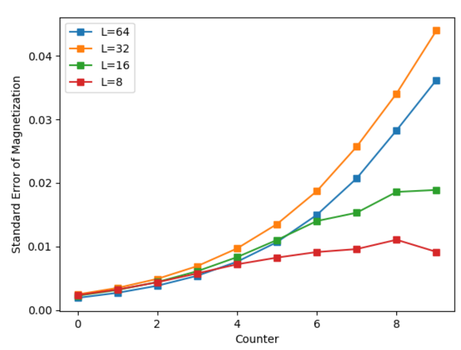


The integrated autocorrelation time defines how many Monte Carlo steps seperate statistically independent spin configurations.

Our learning algorithm then is trained to reduce this time by suggesting a cluster update of the spin configuration resulting in a new, updated spin state that is much less correlated from the initial one compared to the single spin-flip Metropolis algorithm.

Standard Error

As the system size increases, our data becomes less precise. A more efficent algorithm would decrease error by allowing more and longer simulations.



$$\sigma^2 = \frac{1}{B(B-1))}\sum_{b=1}^{B}[\overline{M}_b - \overline{M}]^2$$

The equation given allows us to plot the error for each system size, but our data is not independent, so each line approaches the true standard error.

References:

- A. W. Sandvik, AIP Conf. Proc. **1297**, 135 (2010).
- J Liu, Y. Qi, Z. Y. Meng, L. Fu, Physical Review B **95**, 041101(R) (2017).