Generative Adversarial Network on 2-D Ising Model

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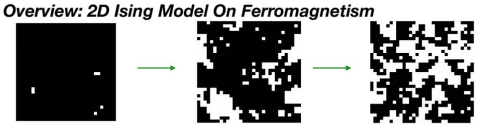
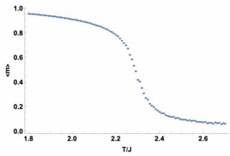
2-D Ising Model: Different Approaches

• Overview: 2D Ising Model On Ferromagnetism



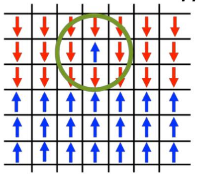
T = 1.5 T = 2.3 T = 3.0

2D Ising Model is an important model on magnetism. The model consists of discrete binaries that denote two states of atomic spin (black square for "+" state and white square for "-" state. The energy of a specific configuration is determined by its Hamiltonian, $H(\sigma) = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j$
where the first summation accounts for the interaction between adjacent squares, and the second summation indicates the external magnetic field.



Let <m> be the average magnetization on a single spin, then both the configurations above and calculated values shown on the left illustrate that if we increase the temperature, the randomness of the system tends to increase, and there exists a very sharp slope at T ~ 2.3 for such increase.

• Traditional Method and Limitation: Metropolis Algorithm and Mean-Field Approach



Metropolis Algorithm on 2D Ising Model treats the whole simulation process as a Markov chain. For each step, we randomly pick a spin to flip its sign. The flip will be automatically accepted if the total energy of the system decreases, and $P = e^{-\Delta E/k_B T}$ to accept the flip if the total energy of the system increases by ΔE.

Limitation:

- Very long simulation for larger system.
- The correlation J is subjected to the change of local spin configurations in many real cases.
- In order to overcome the long simulation time, mean-field approach ignore the correlation between spins, but such method is only valid for dimension larger than 3.
- In solid state physics, there are quite a few strongly correlated 2D materials where mean-field approach fails badly

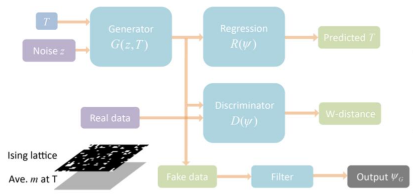
• Generative Adversarial Network: Advantages

The 2D Ising Model can be represented by graphs, as illustrated. GAN is able to generate new figures with given features in the training sets. Thus regarding each spin as a pixel in a real figure, we propose that GAN is able to:

- generate reasonable configurations of a 2D Ising Model at a certain temperature.
- Reproduce the system parameters such as the average spin per particle, and predict if the given configuration is a real configuration at given temperature.

Sampling and Tuning Methods

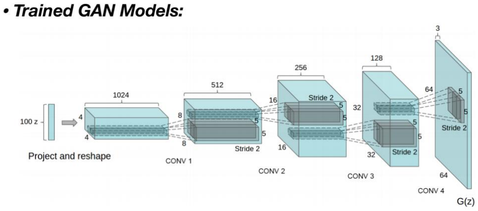
• GAN Architecture of Ising Model Simulator:



Output example

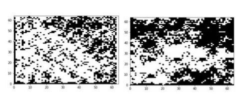
- As shown above[1], two CNNs serve as the discriminator and the regression network, and a transpose CNN acts as the generator. All the CNNs in this framework share the same structure.
- Training data are augmented by adding a second layer of magnetization information at a given temperature T, in order to map the originally overlapped distributions into other dimensions.

• Trained GAN Models:

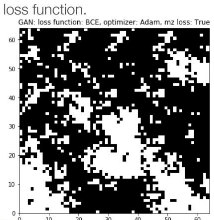


$$\min_G \max_D V(D, G) = \mathbb{E}_{x\sim P_{data}}[\log D(x)] + \mathbb{E}_{z\sim p_z(z)}[\log(1 - D(G(z)))]$$

- **Generator:** as shown above[2], it tries to minimize the probability that the fake images are classified as fake. We adopted the standard DCGAN generator network with a different last layer: a stepping layer was added to set all positive elements to 1, and all negative elements to -1, which correspond to the real Ising spin values.
- **Discriminator:** it tries to maximize the probability that it classifies real images, $x \sim P_{data}$ as real, and fake images $G(z)_{z\sim p_z(z)}$ as fake. The architecture is similar to the generator, with transposed convolution replaced by regular convolution and ReLU activation replaced by leaky ReLU.
- **Training**: mini batches. Dataset was generated by Metropolis.
- **Loss**: In addition, we added the difference between the average spin of generated sample and real sample to the loss function.



Two figures on the top: without mz loss
Figure on the right: with mz loss

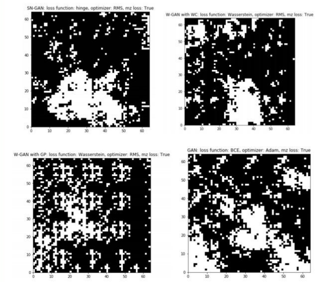


1. Liu, et al. arXiv:1710.04987 (2017)
2. Radford, et al. arXiv:1511.06434 (2015)

Result Comparison

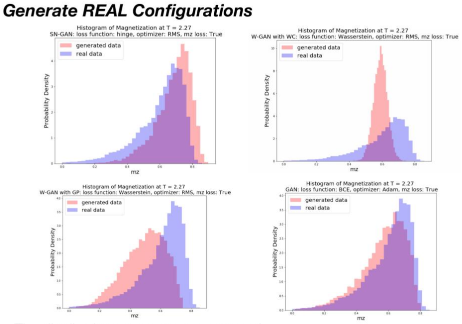
• Reproduce the configurations at critical temperature

Real configuration by Metropolis: the critical temperature configurations of 2D Ising Model tend to show the clustering of the same spin (phase separation).



Configurations generated by four different models. Wasserstein GAN with GP did very poorly on phase separation even with the help of mz loss, and W-GAN with weight clipping improved a bit. The SN-GAN with hinge loss and GAN with BCE loss did a pretty decent job on generating real-life configurations similar to the one above.

• Generate REAL Configurations



- The distributions of mz were compared.
- The discriminator or generator are able to learn that the configurations are randomly generated, but failed to learn its distribution. Even with the help of mz loss,W-GAN with GP or WC still have a hard time learning the distribution.
- With the help of mz loss, SNGAN with hinge loss and BCE loss learned the distribution of the configurations to be Boltzmann. In contrast, other models are only able to learn that the real configurations are random, but not the

• Next step

- Make more learning at different temperature, in order to reproduce the mz vs. T plot from Metropolis.
- Try to tune the hyperparameters in order to learn the long-range correlation between spins far from each other.
- With the ability to learn the long-range correlation, train the model to scale up the size of Ising Model.