Designing Diffusion Models for Ising Systems

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INTRODUCTION

- ➔ Can diffusion models reach the same performance as Monte Carlo methods to generate samples from physical systems?
- ➔ Do diffusion models "react" to the phase transition as naïve Monte Carlo methods do?
- ➔ How much data do we need to train good models?

We answer these questions for the 2D Ising Model.

Why the 2D Ising Model?

- Extensive amount of analytical and numerical results.
- In 2D has a phase transition.
- Usual Monte Carlo methods suffer from a critical slowdown near the phase transition.

Why Diffusion Models?

- Scale well with high-dimensional data.
- Fixed computational cost of generation, unlike Monte Carlo methods.
- State of the art in image generation tasks.

THE 2D ISING SYSTEM

A 2D grid of L×L spins (σ) at temperature T, which can be **up** (+1) or **down** (-1).

Given a configuration $\vec{\sigma}$:

1. **Probability**

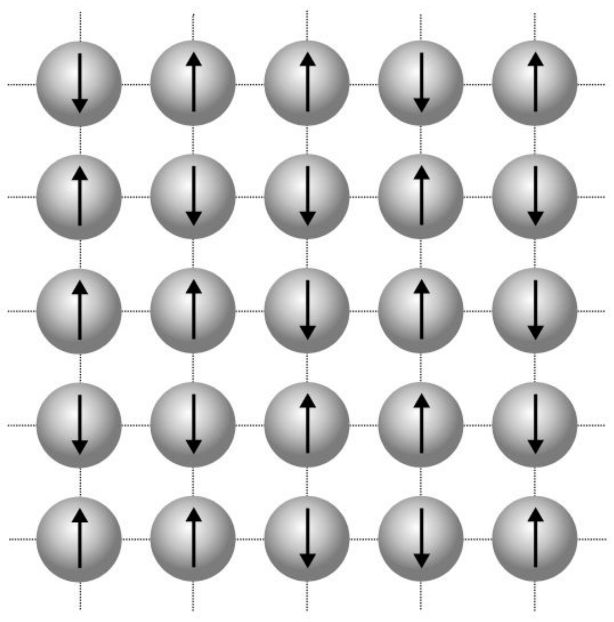
$$P(\vec{\sigma}) = \frac{1}{Z}\exp\left(-\frac{1}{k_B T}H(\vec{\sigma})\right)$$

2. **Magnetization**

$$M(\vec{\sigma}) = \sum_i \sigma_i$$

3. **Energy**

$$H(\vec{\sigma}) = -J\sum_{<i,j>}\sigma_i\sigma_j + h\sum_i \sigma_i$$



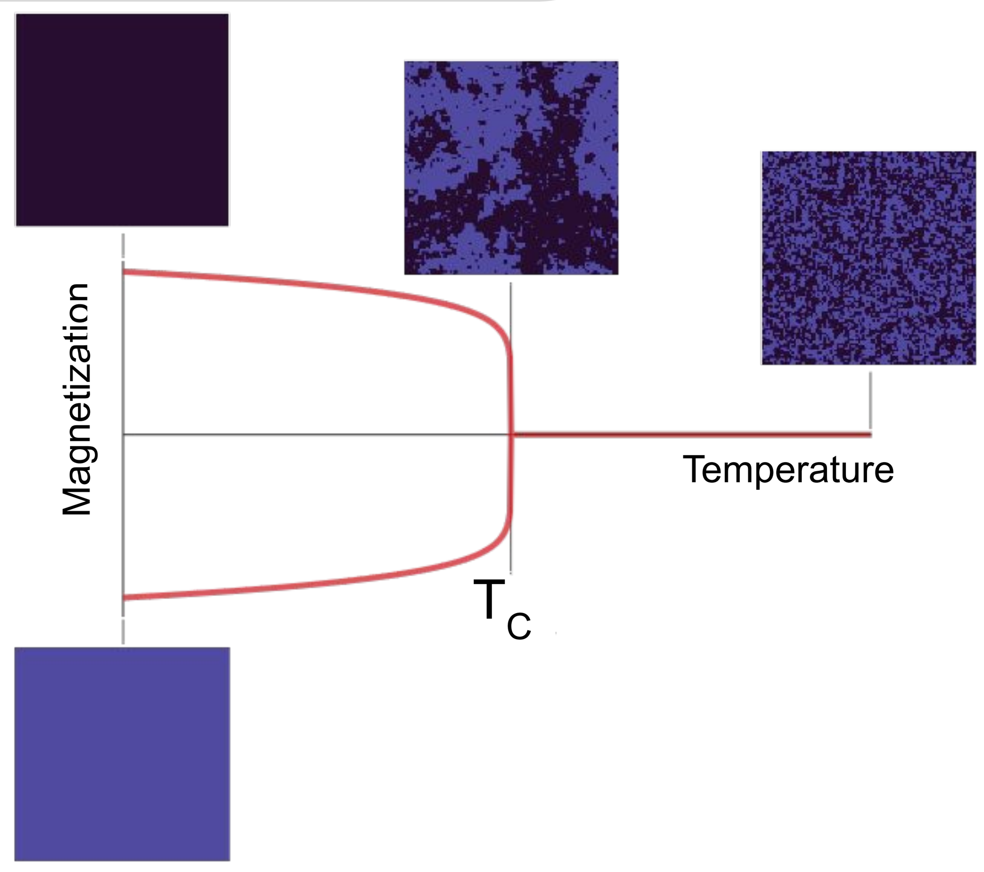
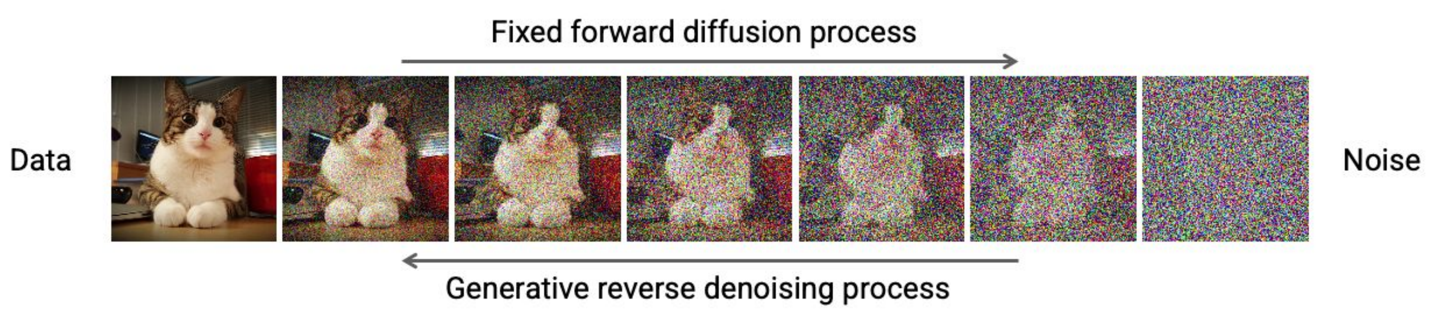
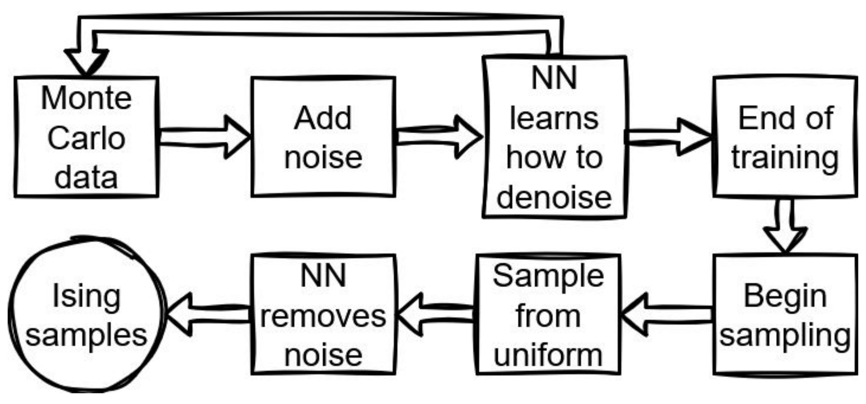


Figure. Samples of the 2D Ising Model at different temperatures. Black is up, blue is down. In red, how the magnetization changes with temperature. The phase transition happens at the critical temperature $T_C \approxeq 2.27$.

DIFFUSION MODELS

- Generative models that can **build samples from noise**.
- We progressively add noise to the training data and train a **neural network (NN)** that learns how to **denoise** samples.



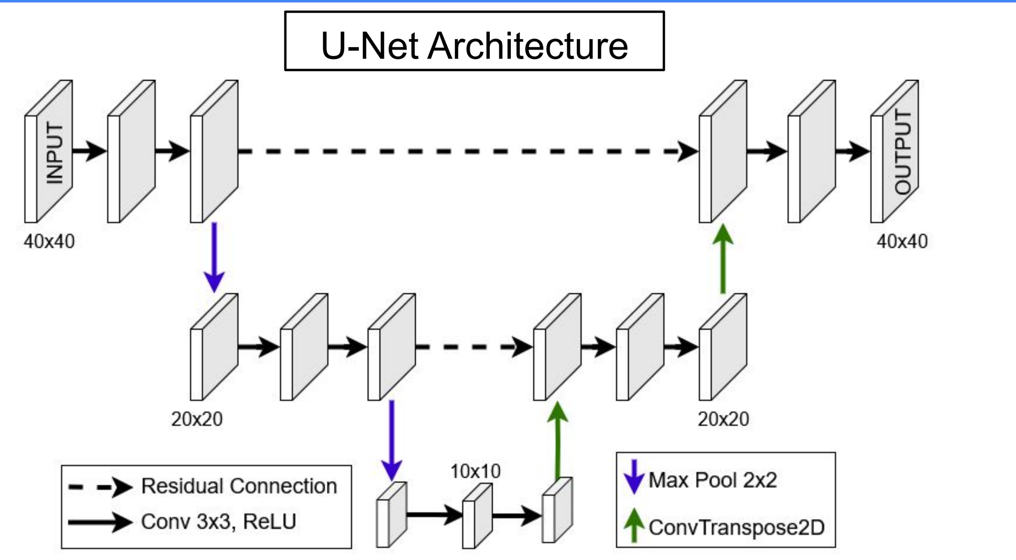


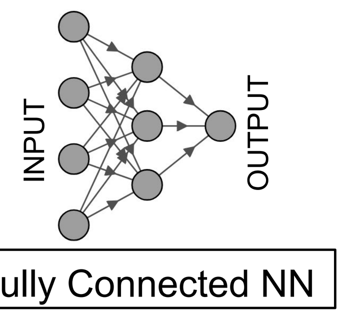
- Implementation works for **discrete state spaces**, like the Ising model, instead of the usual continuous state space [1].

METHODOLOGY

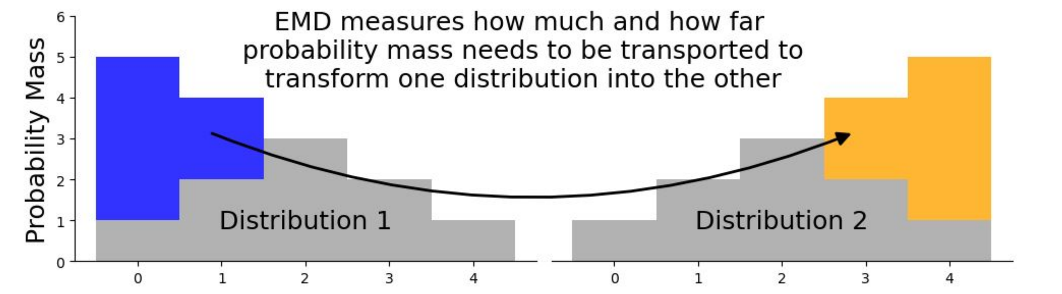
1. Neural Network Architectures:

- **U-Net**, a convolutional NN[2].
- **Fully Connected NNs** where every neuron is connected to every neuron of the next layer.





2. Data Evaluation: Diffusion models' loss is a bad evaluation metric. So we measure distance between energy pdfs using the **Earth Mover's Distance** (EMD).



RESULTS

- At all temperatures, **both networks types are able to replicate the magnetization distribution**.
- However, the **fully connected network fails to replicate the energy distribution** (even if we increase its parameters).

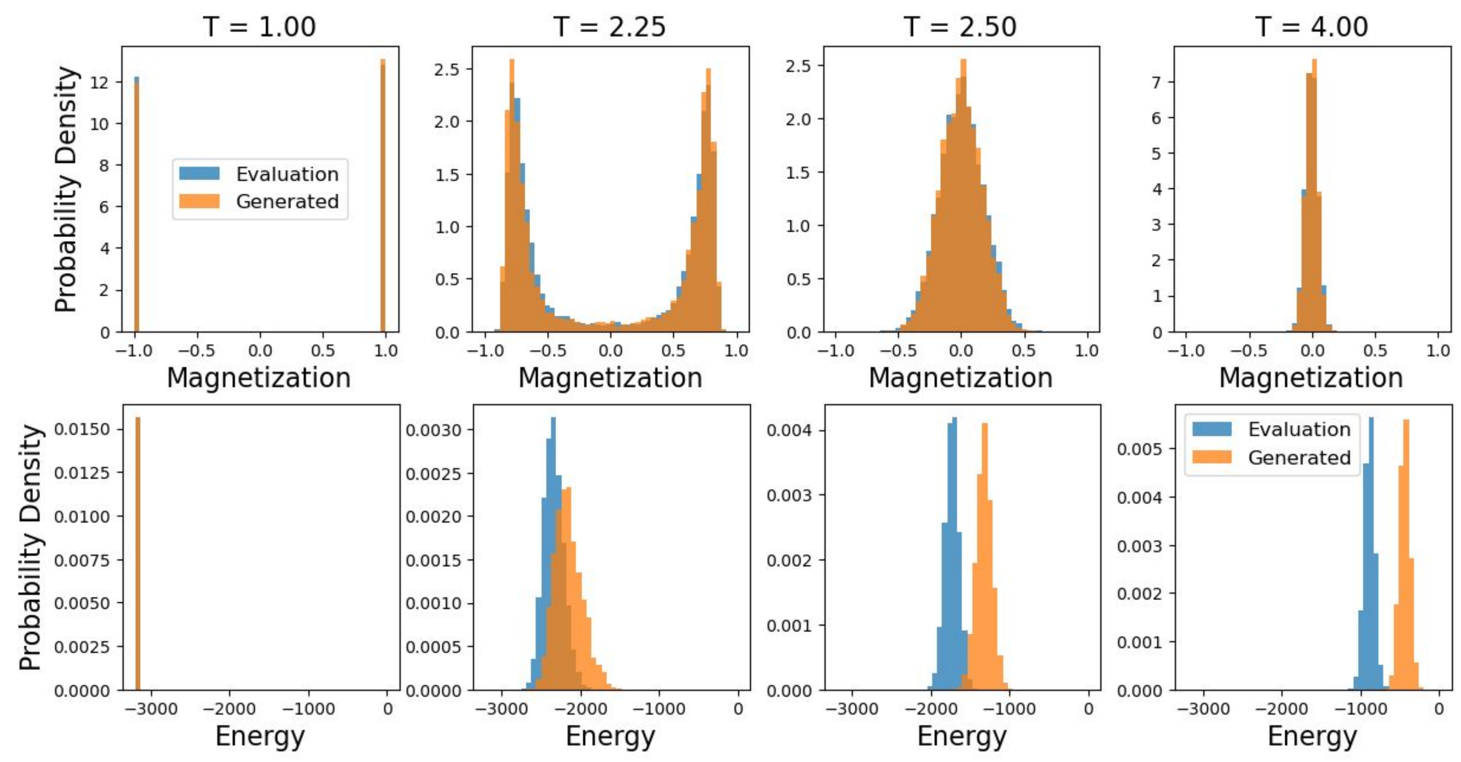
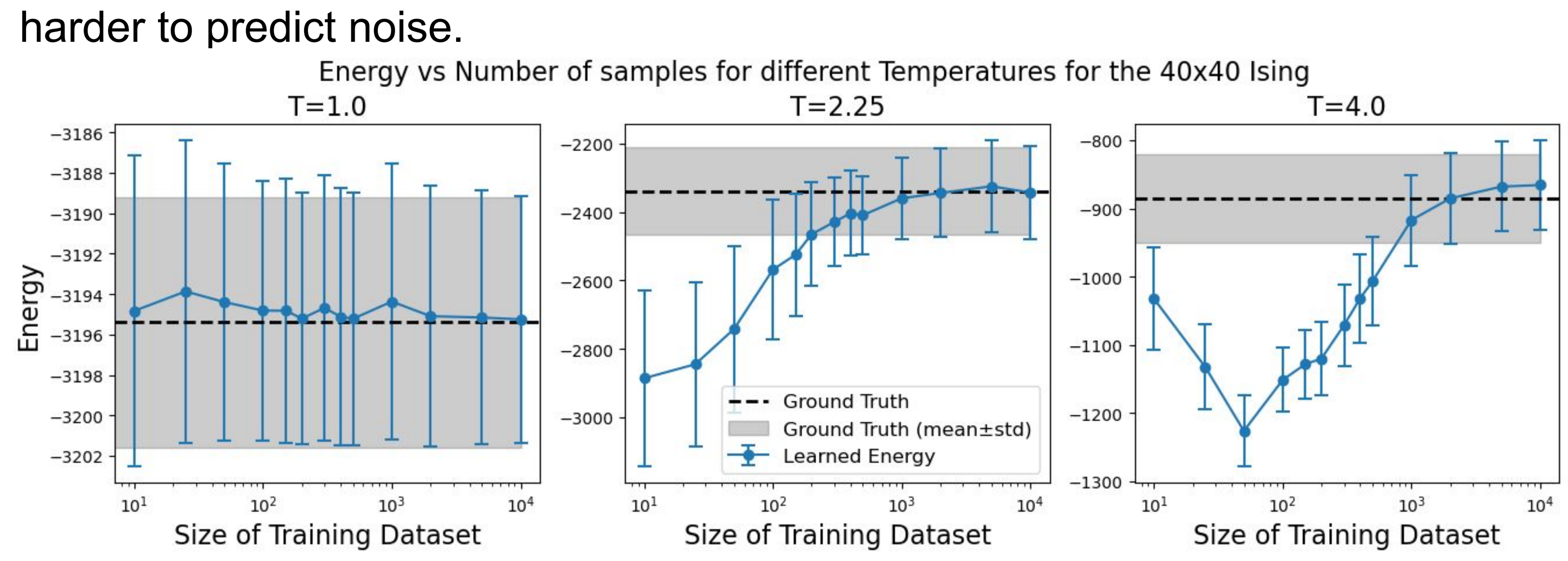
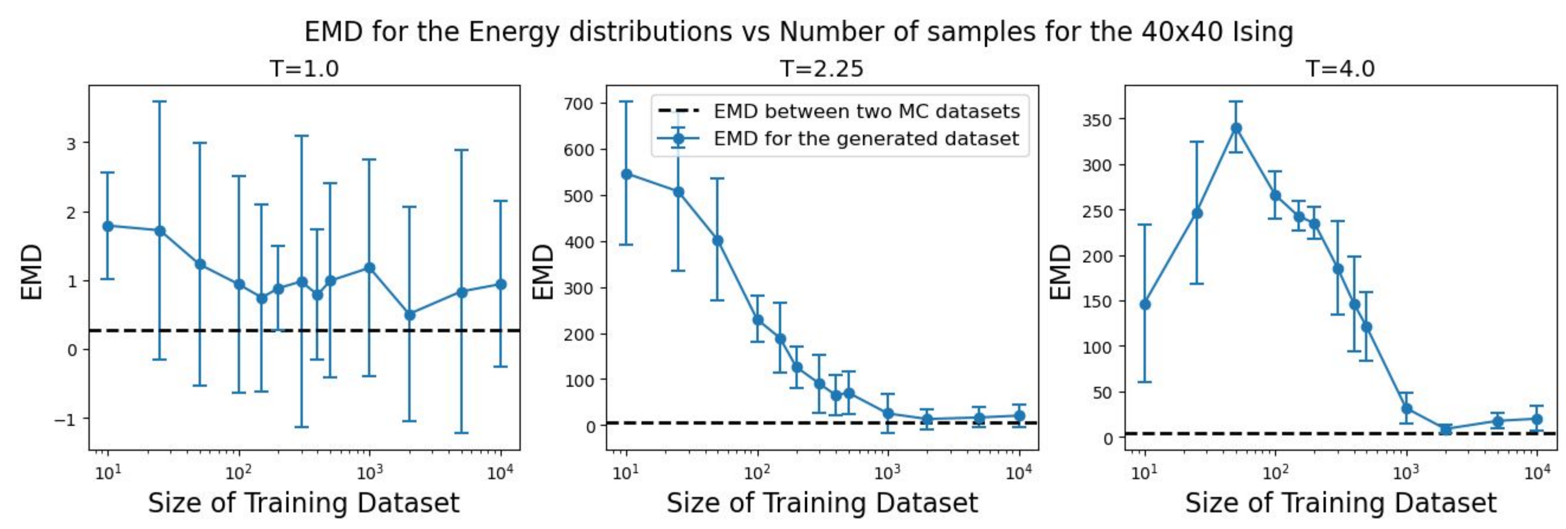


Figure. Magnetization and Energy distributions for the fully connected network.

- **U-Net network can generate samples with similar EMD** as the ones from Monte Carlo methods, if $N_{samples}$>1000, as seen below.
- **Learning gets harder as the temperature increases**, and not only near the phase transition.
- At higher temperatures, there is no discernible pattern in the data, making it harder to predict noise.





FUTURE WORK

- Explore other noising schedules, that instead of converging to the uniform distribution, converge to a single point.
- Train a **conditioned diffusion model**, which accepts the **temperature as an input**, outputting a sample of the Ising model at that temperature. See if the phase transition is correctly modeled.

References:
[1] - Austin, Jacob, et al. "Structured denoising diffusion models in discrete state-spaces." NeurIPS 34 (2021).
[2] - Ronneberger, Olaf et al. "U-net: Convolutional networks for biomedical image segmentation." MICCAI (2015).

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