Variational Autoencoders for Classical Ising Models

Ben Nosarzewski

Introduction

Lattice spin models are used to study the magnetic behavior of interacting electrons in solids. We demonstrate that variational autoencoders (VAEs) can learn to properly sample from the correct distribution of spin configurations across a range of temperatures and capture a phase transition. Generative neural networks produce uncorrelated samples and therefore can offer an advantage over Markov chain Monte Carlo methods which often suffer from long autocorrelation times.

We study the classical nearest -neighbor Ising model:

$$H = -\sum_{\langle ij \rangle} J\sigma_i\sigma_j$$

And the classical XY model:

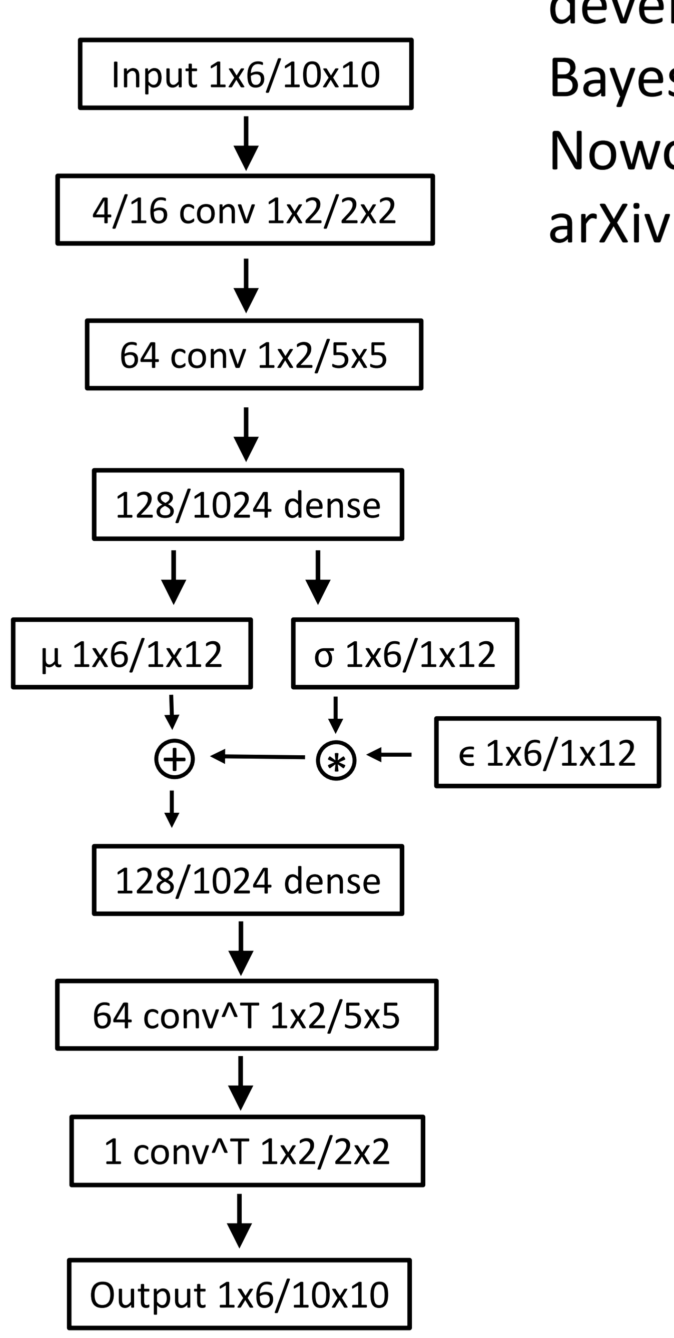
$$H = -\sum_{\langle ij \rangle} J cos(\theta_i - \theta_j)$$

We compute the average energy and the spin-spin correlation function: $\langle \sigma_i \sigma_j \rangle$

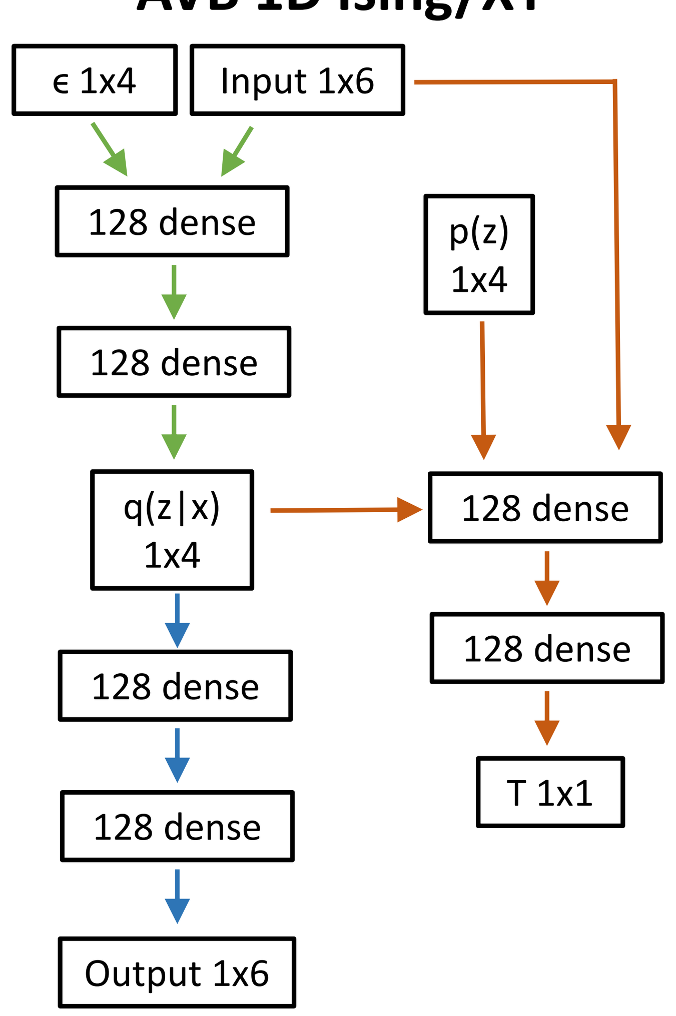
Architectures

Training data is obtained from Markov Chain Monte Carlo using the Metropolis algorithm with single spin updates. The dataset for each temperature consists of 10,000 total samples from 50 Markov chains. In addition to a standard VAE architecture we also use recently developed adversarial variational Bayes (AVB) [L. Mescheder, S. Nowozin, and A. Geiger, arXiv:1701.04722v2 (2017)].

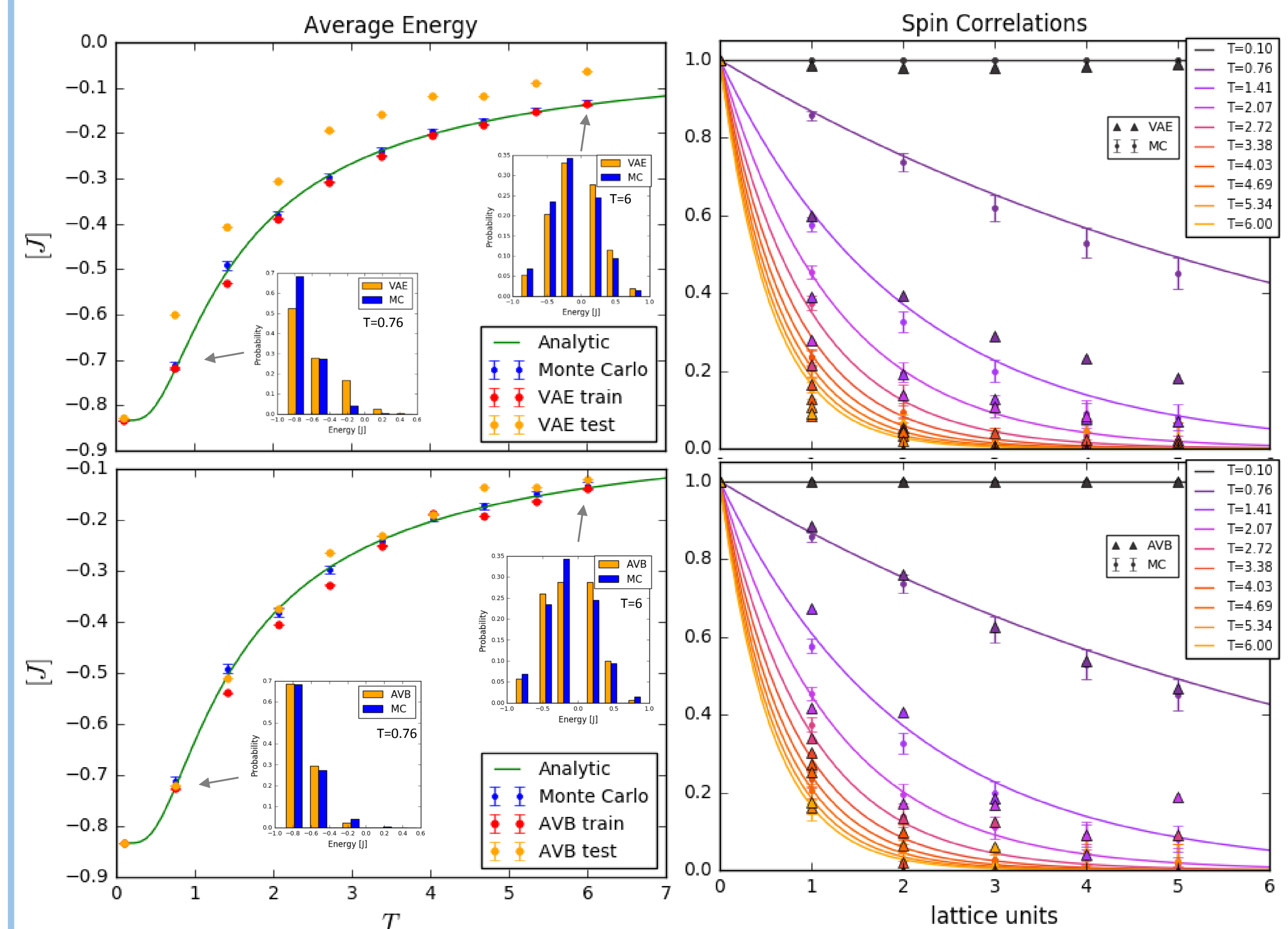
VAE 1D/2D Ising



AVB 1D Ising/XY

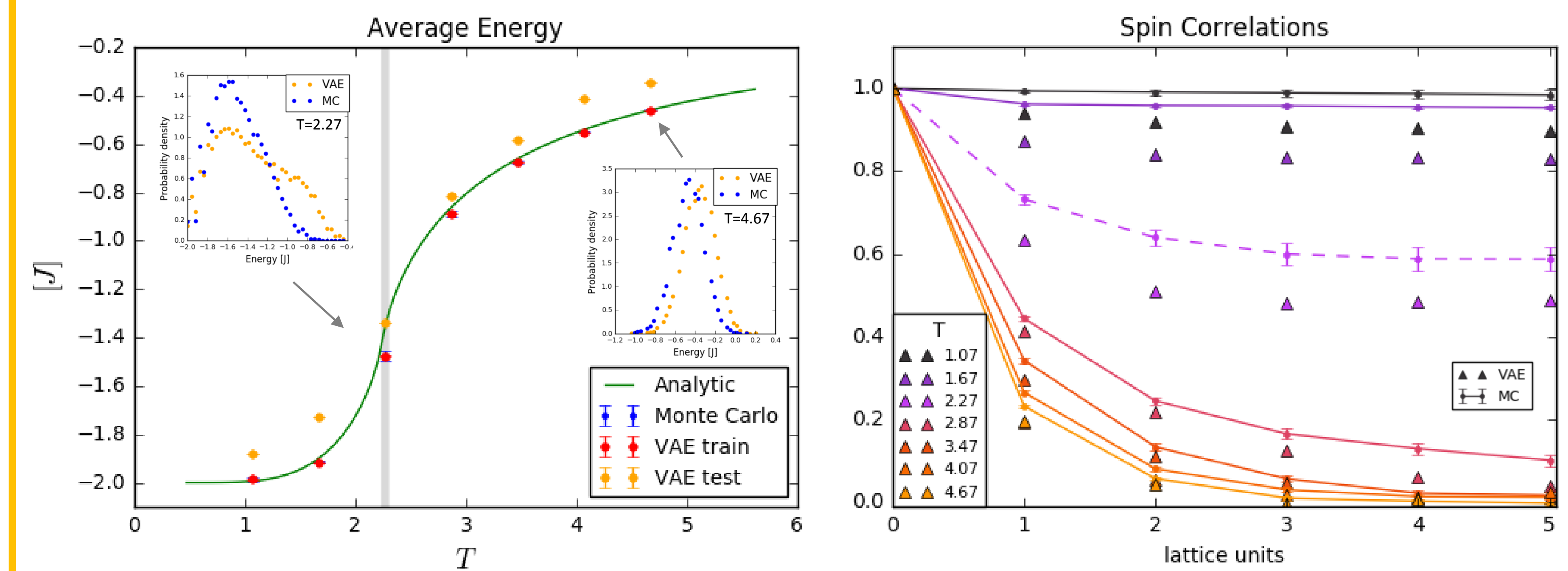


1D Ising Model

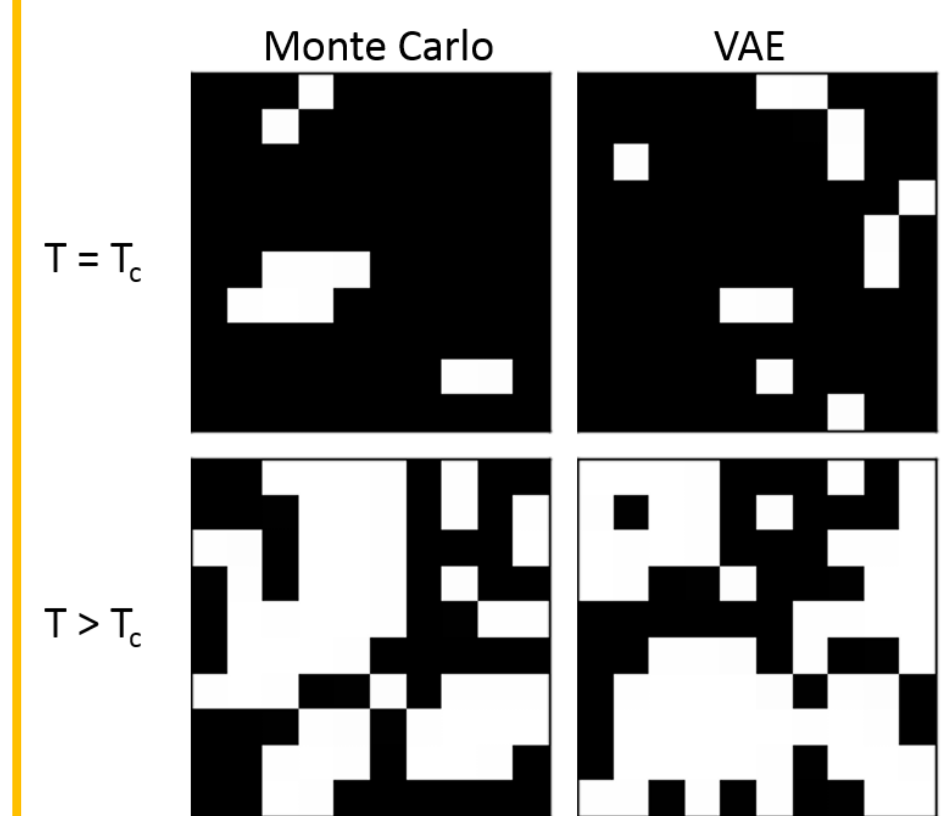


The results above are for a 1D chain with 6 sites with free boundary conditions. Both VAE and AVB capture the average energy, but AVB captures spin correlations better. Solid lines correspond to the exact analytic solution. In the spin correlation figures, triangular markers correspond to results from the neural network while circular markers are for the Monte Carlo. Adding convolutional layers in the VAE improves performance compared to a plain fully-connected architecture. Intuitively, convolutional layers improve performance by detecting domain wall features in the spin configurations which can occur anywhere in the translationally invariant system.

2D Ising Model

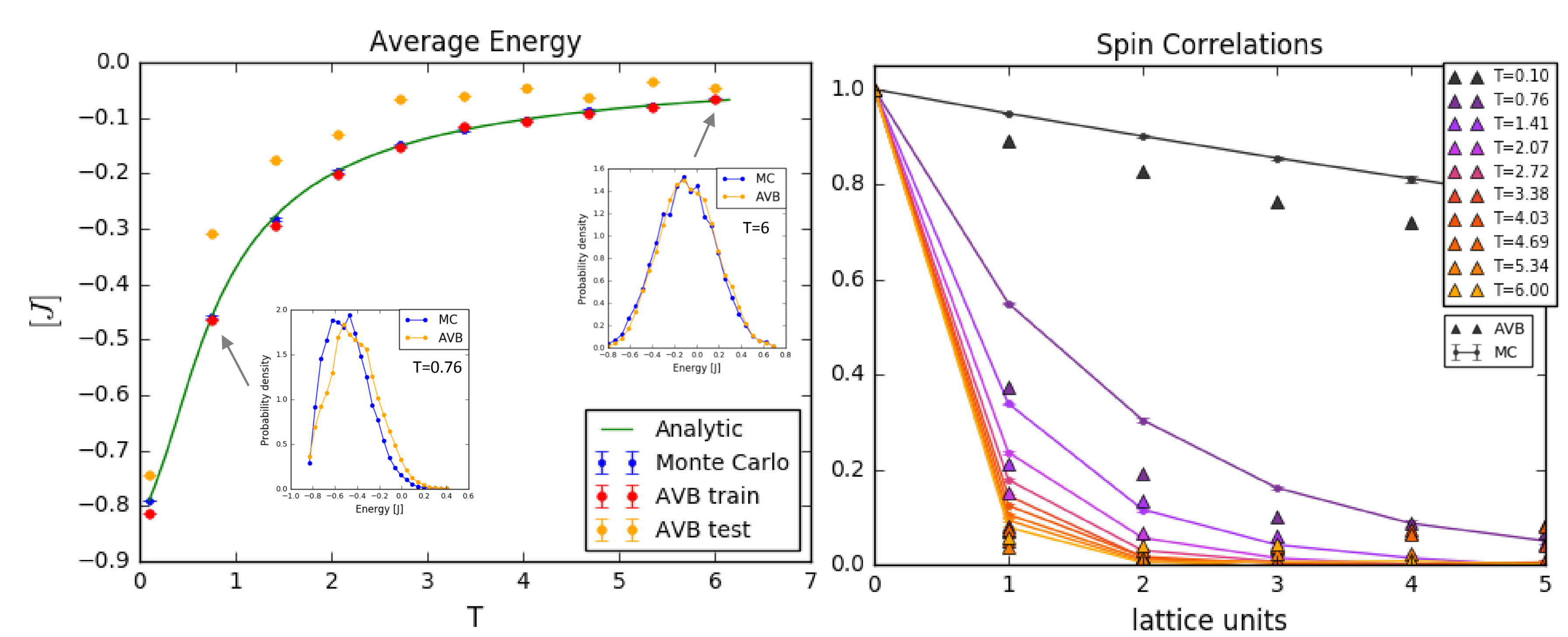


Average energy and spin correlations are captured by the VAE for a 10x10 lattice with periodic boundary conditions. The vertical gray line and dotted magenta line indicate the transition temperature $T=T_c$.



Representative samples chosen with energy equal to the average energy predicted by each method. VAE samples are qualitatively similar to those from Monte Carlo. The comparison is performed at the critical temperature and at the highest temperature in our simulations. Pixel color corresponds to spin up and down. The VAE reconstructs these particular Monte Carlo samples perfectly during training.

1D XY Model



Results for a 6 site chain with free boundary conditions. The XY model differs from the Ising model as it has continuous spin variables. The distribution of states is captured particularly well by AVB as seen in the insets.

Future Work

-Extend AVB to 2D
-Larger lattice sizes
-Study classical XY model in 2D which has a Kosterlitz-Thouless phase transition (2017 Nobel prize)
-Accelerated Monte Carlo
-Frustrated magnetism

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