Denoising Autoencoders for High-Qubit Quantum Dynamics Simulations on Quantum Computers

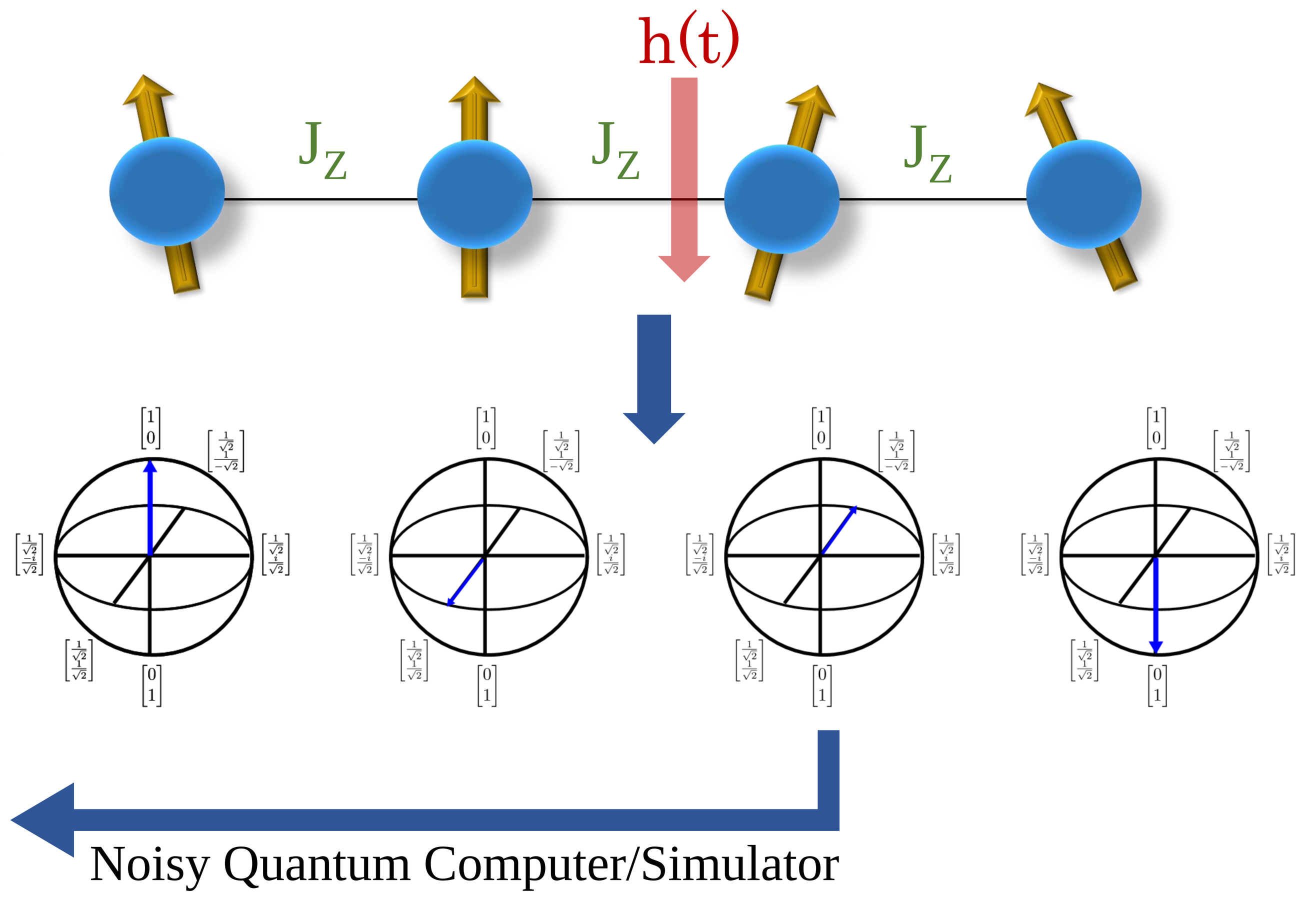
Connor Powers[1], Lindsay Bassman[2], Yifan Geng[1], Rajiv K. Kalia[1], T. K. Satish Kumar[1], Thomas Linker[1], Kuang Liu[1], Aiichiro Nakano[1], Pankaj Rajak[3], Priya Vashishta[1]
[1]University of Southern California [2]Lawrence Berkeley National Laboratory [3]Argonne National Laboratory

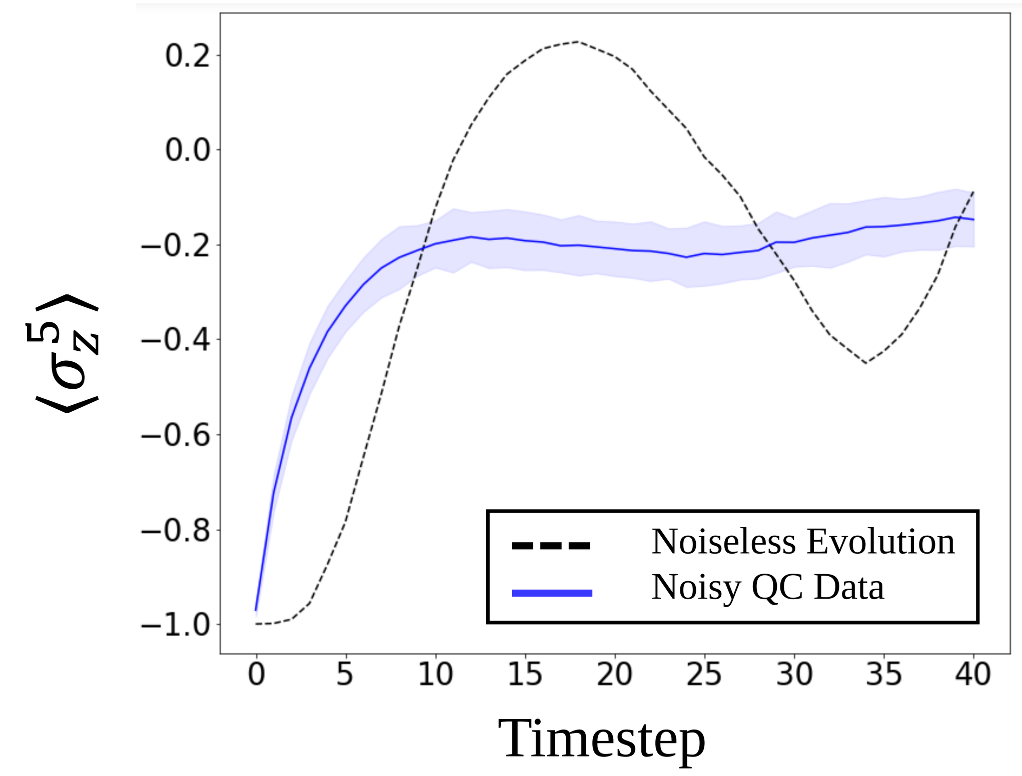
Abstract

Quantum computers hold great promise for discovering new materials behavior by performing dynamic simulations of quantum materials that are intractable on classical computers. However, high-fidelity results from these simulations are currently hindered by high levels of device noise. Here, we present an autoencoder, trained with quantum simulations of small systems, that is capable of filtering noise from dynamic simulations of larger systems run on quantum computers. We thus show a lightweight and feasible route for higher-fidelity quantum simulations of large systems beyond points of classical intractability.

Simulating TFIM Dynamics on Quantum Computers

$$H(t) = -J_z \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - h_x(t) \sum_{i=1}^{N} \sigma_i^x$$



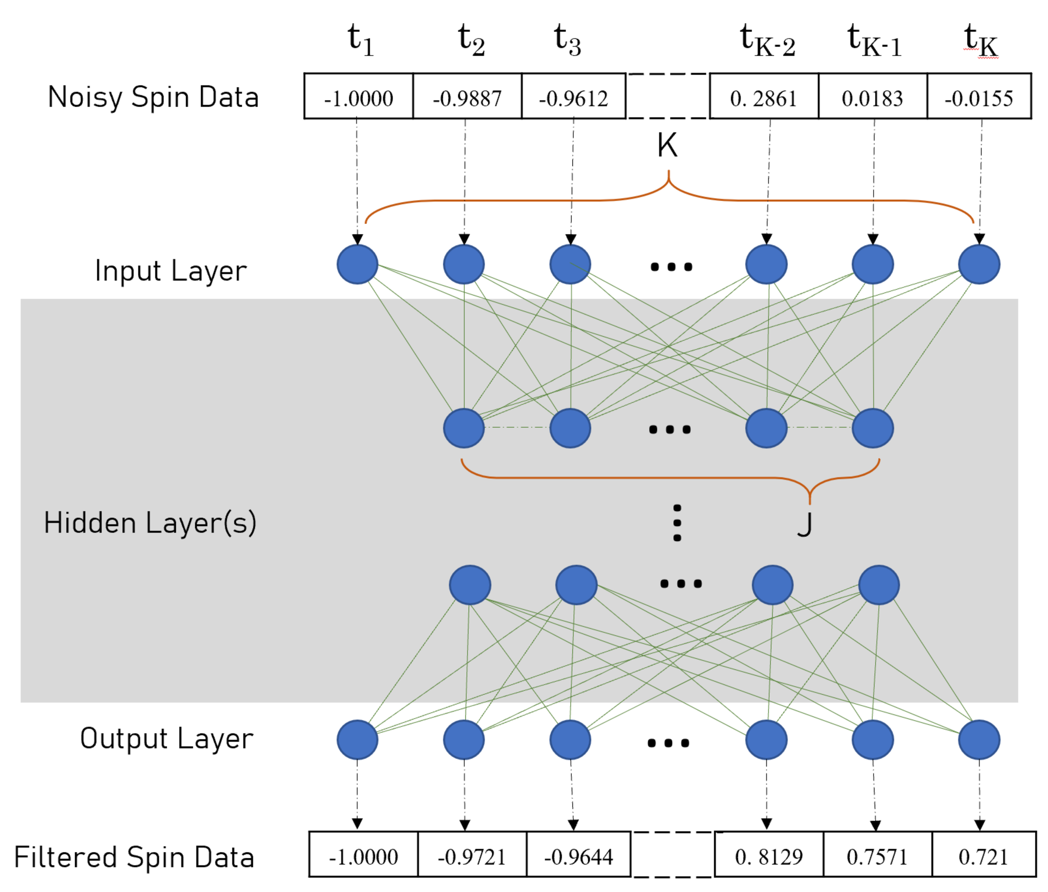


Per Bassman et al., *Phys. Rev. B* **101** 184305 (2020)
and Bassman et al., *Quantum Sci. and Tech.* (2020)

Denoising Autoencoders: Structure and Training

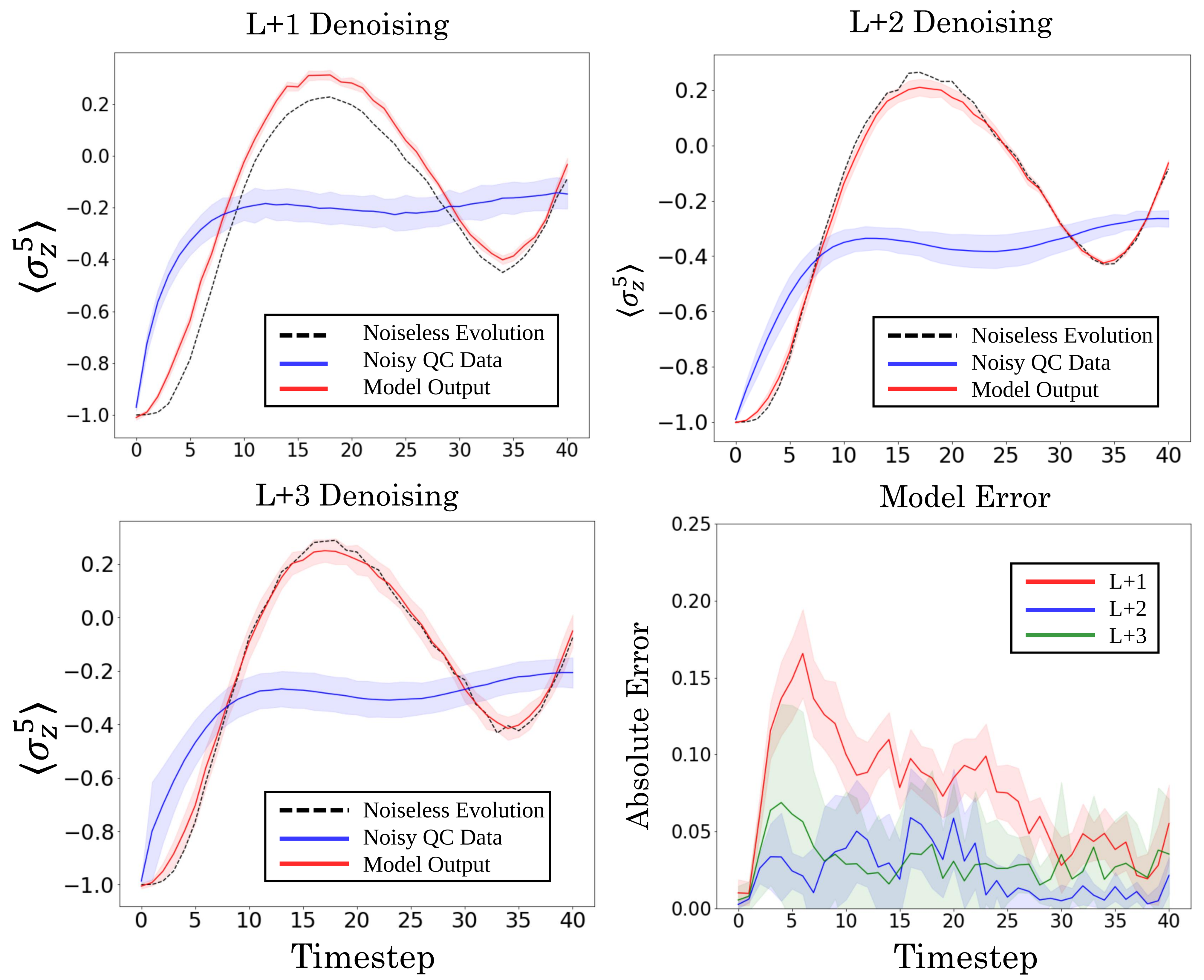
Efficacies of both shallow and deep denoising autoencoders were tested in the denoising extrapolation task. Time was encoded as a spatial dimension, fixing the input feature length *K*. The hidden vector length *J* and percentage of applied dropout to each hidden layer were kept as variables. We found that both shallow and deep variants could satisfactorily filter noise from larger simulations than trained upon, but present the smallest successful networks for practicality purposes, so displayed results are from shallow networks.

The models were trained with the ADAM optimizer with a learning rate of 0.001 and MAE as the loss function, but models were evaluated with Mean Maximum Error to better identify successful models in the context of quantum dynamics simulations.



Results

Performance of an autoencoder trained on TFIM quantum dynamics simulations of up to L=9 spins, then tasked with denoising TFIM dynamics simulations of 10, 11, and 12 qubits. The autoencoder used below has a single hidden layer of J=10 with 20% dropout, is trained for 500 epochs on a training set of 500 simulations, and is tested on a set of 100 simulations for each simulated spin count.



The model is able to filter the higher-qubit noisy quantum dynamics simulations, and does not show degradation in performance when extrapolating to simulations of up to 3 more spins.

Conclusions and Outlook

We have demonstrated the ability of denoising autoencoders to successfully perform the extrapolation task of filtering noise from quantum simulations involving higher spin counts than those trained upon. Specifically, we found that autoencoders trained on 5- to 9-spin simulations were able to successfully filter noise from 10-, 11-, and 12-spin simulations without significant degradation in performance with increasing system size. This analysis was done with simulated quantum computer noise from the Qiskit API, and we are currently extending this analysis to real quantum computer data.