Project 34: QML for reduced order density matrix time propagation

Siheon Park, I-Chi Chen and Das Pemmaraju

Introduction: Our goal is to predict the time evolution of a reduced density matrix (RDM) of a subsystem using quantum machine learning. To this end we are using the Deep Quantum Neural Network (DQNN) [1] architecture as a base model to learn arbitrary open quantum systems. We have managed to implement a numerical model of DQNNs using 'qiskit quantum_info' package as well as the unique unitary update rule developed in Ref. [1], which assembles backpropagation in neural networks. This implementation allows us to classically train the model very fast by not actually computing the gradient at every step. Meanwhile, we have also implemented the circuit-based DQNN model with 'qiskit QuantumCircuit' instance, which would be more practical for NISQ era.

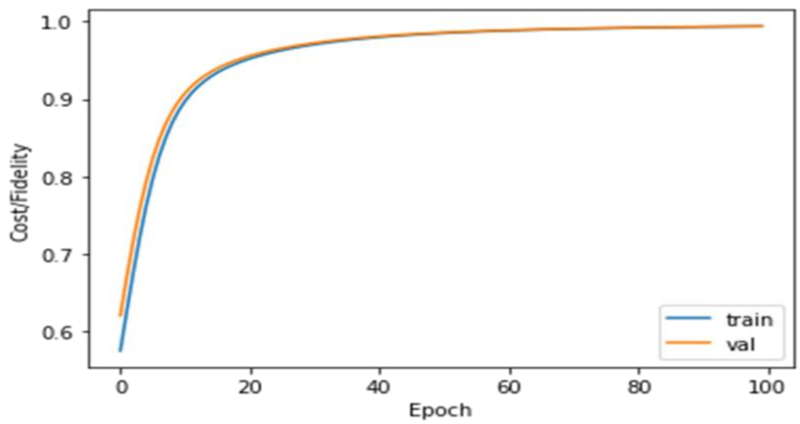


Fig. 1: Training of DQNN

Using the above DQNN (Deep Quantum Neural Network) [1] as the machine learning architecture, we aim to predict the time evolving RDM for a for various instances of the 1D Heisenberg model. We used exact diagonalization (ED) to create a time series of RDMs representing our training and validation data sets.

Results: With the initial state as a trivial product state, in fig.1, we successfully trained a [1,4,1] DQNN model featuring 1, 4, and 1 qubits in the input hidden and output layers respectively and get the training loss function (average fidelity) and validation loss function (average fidelity) to converge to 1 after 100 epochs. We can also predict the expectation value of X, Y, Z Pauli matrices. The result of the prediction is very close to the result from ED shown in fig.2.

For product starting states we also investigated the effect of going beyond a Markov assumption by incorporating an RDM history into the input to our DQNN. Accordingly, we have successfully predicted the quantum state of a qubit in the Heisenberg chain, by observing few (1~3) past states of that qubit (Fig 3). The model with Markovian assumption was equally accurate as the model without for the starting states considered. We further observed that the trainability of DQNN on open quantum system is dependent on the initial state.

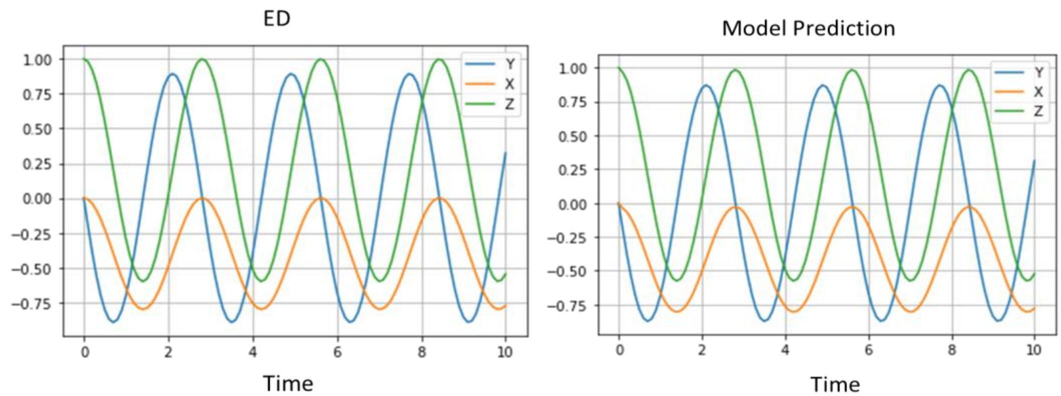
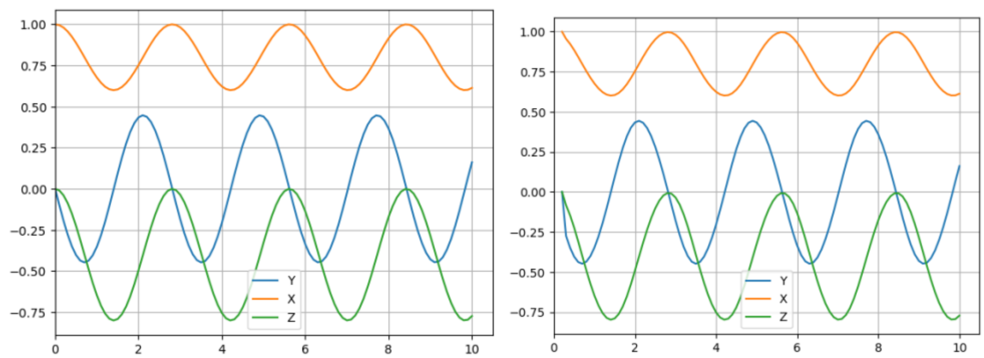


Fig.2 Exact and predicted Bloch vector dynamics for a single site form the 1D Heisenberg chain



Ground-Truth Bloch vector Estimated Bloch vector

Fig.3 Exact and predicted Bloch vector dynamics for a single site form the 1D Heisenberg chain including non-Markov history dependence

Future work: We plan to test our circuit implementation of the DQNN in the coming days and assess performance relative to classical matrix based approaches. Moreover, we will try different models to explore the limitations of this DQNN architecture. We hope to test some non-integrable models which potentially depolarize the reduced density matrix.

[1] Beer, Kerstin, et al. "Training deep quantum neural networks." Nature communications 11.1 (2020): 1-6.