Improving the Use of Neural Differential Equations for Quantum Many-Body Hamiltonian Learning with Classical Shadows

The Hamiltonian Learning (HL) problem consists of the task of inferring the Hamiltonian of a many-body system given a set of state trajectories of that system. The problem is highly relevant for error mitigation, optimal quantum control, quantum simulation, and device certification ([1], [2], [3]). In [4], T. Heightmann et al. introduced a novel approach to solving the HL problem on quantum many-body spin systems using neural differential equations (NODEs). Their proposed method combines an Ansatz Hamiltonian with NODEs to infer the quantum dynamics of a many-body system. The authors showcased the reliability and expressiveness of their method by solving several previously unsolved HL problems in one-dimensional spin-1/2 chains. However, the loss function used to train the parameters θ for both the Ansatz Hamiltonian and the neural network is calculated as the average negative log-likelihood of the probabilities $|\langle b|\psi_\theta(t)\rangle|^2$ using Born's rule for the bitstrings b in a subset of the given dataset corresponding to all bitstrings measured at the same timestamp and input state as the estimator $\psi_\theta(t)$. Despite several other challenges, the authors highlight that such a loss function relies on an accurate estimate of the log-likelihood of a small number of Pauli strings. This could bias the loss function if the number of measurement bases is insufficient or measurements are noisy. At the same time, the authors note the possibility of using classical shadows introduced in [5] to eliminate these disadvantages.

In this project, we will elaborate on this idea by modifying the loss function by tracking expectation values in time using classical shadows. We will do this by generating classical shadows for the evolved states $|\psi_\theta(t)\rangle$ and calculating a new loss function on that basis. We start with randomized measurements by applying random unitary transformations to the quantum state $|\psi_\theta(t)\rangle$ and measure the transformed states to obtain a series of bitstrings $|b\rangle$. Afterwards, we reconstruct for each bitstring an estimator $\hat{\rho}_i$ for the density matrix $\rho_\theta = |\psi_\theta(t)\rangle\langle\psi_\theta(t)|$ using the relation $\hat{\rho}_i = M^{-1}(|b\rangle\langle b|)$ with the measurement protocol M. To obtain an estimator for the entire density matrix $\hat{\rho}_\theta$, we form the ensemble mean over the various estimators $\hat{\rho}_i$. Using $\hat{\rho}_i$ we are able to estimate the probabilities for arbitrary bitstrings b with $p(b|\psi_\theta(t)) = \mathtt{Tr}(\hat{\rho}_b\hat{\rho}_\theta)$ where $\hat{\rho}_b = |b\rangle\langle b|$. We obtain our desired new loss function by summing up the negative log-likelihood for all bitstrings measured at the same time step and input state as $|\psi_\theta(t)\rangle$.

We expect the method in [4] using our new loss function to have numerous advantages over using the old one. In particular, we expect that the two challenges mentioned in [4] can be resolved. The limited coverage of Pauli bases can be overcome using classical shadows, which enable more accurate reconstruction of the probabilities $|\langle b|\psi_\theta(t)\rangle|^2$ by aggregating data across different random measurement bases, while their randomized nature ensures uniform Hilbert space sampling and mitigates biases from restricted measurement bases. Also, classical shadow protocols are designed to be robust against certain types of noise [6]. For example, we could use error-mitigation techniques to correct systematic errors in our measurements [7].

To explore the benefits of the new loss function, we aim to implement the algorithm with our modified loss function and benchmark it against the algorithm using the old loss function from [4]. We do this in three steps: First, we familiarize ourselves with the current algorithm proposed in [4] and try to reproduce the results for the 1-dimensional quantum systems mentioned. Second, we change the loss function used in [4] and implement the calculation of our new loss function using classical shadows, as described in the previous section. Finally, we benchmark the performance of the algorithm on the same 1D spin-1/2 chains in [4] for $N \in \{3, \ldots, 8\}$. In particular, we have a close look at systems with only a few measurement bases and with noisy measurements. If time allows, we would also apply the method in [4] to several HL problems in 2 dimensions starting with the 2-dimensional Ising model, both with the old and the new loss function.

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