Bootstrapping Classical Shadows for Neural Quantum State Tomography

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Accessing experimentally prepared quantum states is obstructed by the limited rate at which classical information can be extracted from a quantum state through costly repetitive quantum measurements. It is therefore imperative to treat the *quantum data* collected from quantum experiments as scarce, highly valuable information and to maximize its utility. The quantum data must be stored in a classical data structure as a proxy for future access to information about the quantum state. In the simplest case, this data structure is the list of all the measurements performed (e.g., a tomographically complete set of measurements such as the classical shadow measurements [1]). In principle, such a raw dataset already includes all the information that has been collected from the quantum state. This raises the question as to what the role of a neural quantum state is when it cannot learn more about the physics of the quantum state than what it is provided in the form of training data. However:

(a) the amount of memory required to store a tomographically complete set of measurements grows exponentially with the size of a quantum system;

(b) using this raw data to estimate various observables of the system may result in highly erroneous and often unphysical estimations; and

(c) every such estimation requires sweeping over the exponentially large list at least once.

Maximum likelihood estimation offers a path to alleviating all these challenges using memory-efficient parameterized models (i.e., ansatze). Model parameters are variationally optimized in update directions that make the training data most likely to be generated by the learned ansatze. Such variational ansatze can flexibly be used to impose physicality on the reconstructed states. Among various approaches, tensor and neural networks provide flexible architectures capable of capturing relevant regions within the Hilbert space. Moreover, when these networks possess an autoregressive property, they can efficiently provide independent samples for subsequent tasks downstream as generative models for the learned quantum states.

Recently, Ref. [2] proposed an approach for training a neural quantum state using classical shadows, to combine the advantages of variational anstaze and classical shadow measurements. The authors introduce the infidelity between the classical shadow state (introduced in [1]) and the ansatz as their loss function, enabling its training on Clifford measurements. However, because the classical shadow states can be unphysical, infidelity is not constrained within the physically valid $[0, 1]$ range. Additionally, infidelity cannot guarantee bounded errors in approximating many quantities of interest from the trained model and it does not generalize to a training loss function for ansatze of mixed states. Finally, Ref. [2] uses a pretraining strategy in its training protocol that uses prior knowledge about the state, without which the infidelity-based optimization stalls.

In this paper, we investigate the advantages of using autoregressive neural quantum states as ansatze for classical shadow tomography to improve its predictive power. We introduce a novel

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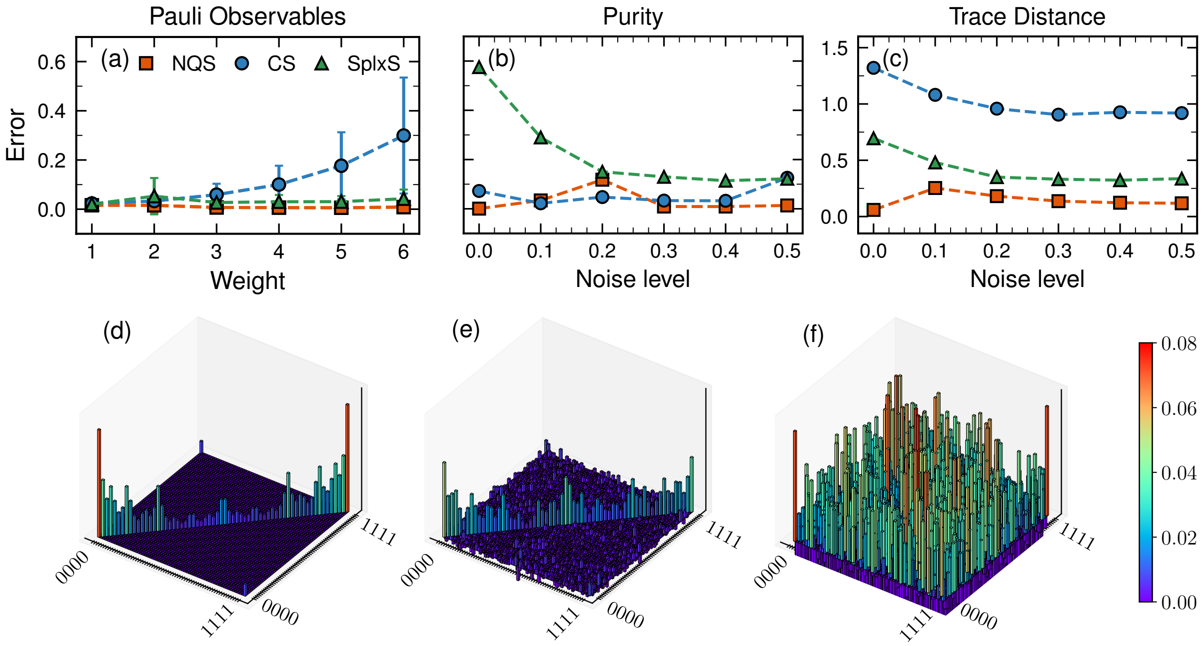

FIG. 1. Comparison of the predictive capabilities of neural network quantum states, classical shadows, and the simplex projection of the latter, for high-weight Pauli observables and purity. A six-qubit GHZ state affected by a depolarizing noise channel of various levels $p \in [0.0, 0.5]$ is numerically simulated and 5000 classical shadows are collected. (a) Absolute error, ϵ, in predicting random Pauli observables of the noisy state averaged over noise levels ranging from $p = 0.0$ to $p = 0.5$ with standard deviations represented by error bars. (b) Absolute error in predicting the purity of the noisy states across the same various noise levels. (c) The reconstruction error of each method in trace distance, averaged across the same noise levels. (d)–(f) Values of real components of the density matrix elements for the noise level $p = 0.5$, comparing the ideal case (d), the neural quantum state (e), and the classical shadow state (f). The colour bar indicates the magnitude of each component of the density matrix.

estimator for optimizing the cross-entropy loss function using classical shadows, and a new importance sampling strategy for estimating the loss gradient during training using stabilizer samples collected from classical shadows. This loss function also enables the training of neural quantum states representing purifications of mixed states. The main contributions of our paper are as follows.

1. *New loss function.* We provide a novel estimator for the cross-entropy loss function using classical shadows. This loss function is viable for training mixed states.
2. *New importance sampling strategy.* We introduce *stabilizer-based* sampling for estimating the overlap between classical shadows and a neural quantum state. This overcomes the need for pretraining and significantly reduces the variance of gradient estimations during training.
3. *Supervision of a physically valid mixed-state autoregressive model on measurement data.* We show that our new loss function can be used to train a neural network representing a purification of the mixed quantum state from classical shadow training data.
4. *Superior prediction of high-weight observables compared to raw classical shadow estimations.* We show that the physicality constraints natively imposed by the explicit access of autoregressive models to conditional probability densities (in the autoregressive expansion) improve the accuracy of predictions extracted from classical shadow data.

We use numerical simulation of pure and mixed GHZ states to demonstrate the advantages of our approach as summarized in Fig. 1. Since in any relevant experimental setup the states to be studied and characterized are mixed, we use a six-qubit GHZ state depolarized according to various channel strengths to highlight the significance of our techniques for experimentalists. We note that Clifford measurements require deep circuits to implement Clifford twirling, which is not feasible on noisy quantum computers. To overcome this challenge, *shallow shadow* protocols have been devised [3–6]. The depth of the Clifford decomposition prescribes an upper bound on the weights of the observables that can be estimated well using the collected measurements. In contrast, the generalization power of our natively physical ansatz allows us to use the "shallowest" possible Clifford tails (i.e., Pauli measurements) to achieve satisfactory predictions of high-weight Pauli observables as well as nonlinear observables such as purity.

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