CLASSICAL SHADOW METHOD VERIFICATION AND MACHINE LEARNING OF A SIMULATED QUANTUM SYSTEM

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ABSTRACT

This report will mainly discuss the paper *"Provably efficient machine learning for quantum many-body problems"* [1]. In this paper [1], the author used a method called *Classical Shadow Representation*, which is the main work in another early paper [2] by same author. We will show the performance of classical shadow representation, and also train a model which tries to learn to predict classical shadow representation of a given quantum system.

All of the source code written by us can be found at `https://github.com/r08222011/Quantum_Classical_Shadow_ML`.

Keywords Quantum Computation, Classical Shadow Representation, Machine Learning

1 Introduction

Quantum computation science and technology has becoming a popular research field. But doing quantum simulation or quantum experiment might cost a lot of time and money, or even impossible to do simulation. Due to the limitation of experiment resources, one might want to predict the property of a material or a quantum system with the data from experiments done already. In the work of [1], the author shows that one can learn quantum many-body systems efficiently with classical machine learning method.

Suppose we have a n-qubit quantum system, sometimes it is hard to do quantum tomography to reconstruct the original quantum state efficiently. In the early work of [2], the author shows that one can use *Classical Shadow Representation* to reconstruct the approximated density matrix of a quantum system. In [1], the author showed that one can use classical machine learning to learn a model which can efficiently (compare to classical methods without data) predict the approximated density matrix. One then can use the predicted density matrix to predict the property of a quantum system.

This report will be organized in the following: In section 2, we will briefly introduce the *Classical Shadow Representation* method in [1][2][3]. In section 3, we will demonstrate the performance of classical shadow representation method. We also trained a simple neural network to learn a randomly generated quantum circuit as if it were some quantum system. In section 4, we will give a summary.

2 Problem and Methodology

2.1 Classical Shadow Representation

Suppose we have a n-qubit system, it requires at least $O(2^n)$ to store the whole information of its quantum state. Furthermore, if we do not know the exact evolution of the system, it would be costly to do quantum tomography. *Classical Shadow Representation* allows us to represent the density matrix of the quantum system in a more efficient way. The steps are the following:

(i). Suppose the true (unknown) quantum state density is ρ, and we are able to prepare T copies of ρ.

(ii). For each copy, measure each qubit in a randomly selected basis of X, Y or Z. For example, one can measure qubit 1 in Y basis, qubit 2 in Z basis, etc. Finally, each qubit will be in a state of $\{|0\rangle, |1\rangle, |+\rangle, |-\rangle, |i\rangle, |-i\rangle\}$. For the t-th copy of ρ, the i-th qubit measurement outcome basis will be denoted as $\left|s_i^{(t)}\right\rangle$, with $i \in 1, 2, 3, ..., n$ and $t \in 1, 2, 3, ..., T$.

(iii). Reconstruct the approximated density matrix as

$$\rho \approx \sigma_T(\rho) = \frac{1}{T}\sum_{t=1}^{T} \sigma_1^{(t)} \otimes \sigma_1^{(t)} \otimes ... \otimes \sigma_n^{(t)} \quad \text{where} \quad \sigma_i^{(t)} = 3\left|s_i^{(t)}\right\rangle\left\langle s_i^{(t)}\right| - \mathbb{I} \tag{1}$$

Due to the magic number 3 in front of $\sigma_i^{(t)}$, we get $\mathrm{Tr}\left(\sigma_i^{(t)}\right) = 1$. Since $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A)\,\mathrm{Tr}(B)$, we have $\mathrm{Tr}(\sigma_T(\rho)) = 1$. This classical shadow representation has been shown [2][3] to reproduce the global density matrix in the limit $T \to \infty$.

2.2 Hilbert-Schmidt inner product and Frobenius norm

In the next section 3.1, we would like to test the performance of classical shadow representation $\sigma_T(\rho)$ with two quantities, known as *Hilbert-Schmidt inner product* and *Frobenius norm*.

Consider two density matrix A and B. We calculate their Hilbert-Schmidt inner product by $\langle A|B\rangle = \mathrm{Tr}\left(A^\dagger B\right)$. And we also calculate their Frobenius norm of difference as $||A - B||_2 = \mathrm{Tr}\left((A-B)^\dagger(A-B)\right) = \langle A - B|A - B\rangle$, which is just the Hilbert-Schmidt norm of $A - B$. Intuitively speaking, if A is approximated equal to B, their Hilbert-Schmidt inner product $\langle A|B\rangle$ should be close to 1, else 0. Also their Frobenius norm of difference should be close to 0. We will show the detail of testing performance of classical shadow representation with these quantities in 3.1.

2.3 Predicting density matrix of quantum systems

In the original paper [1], the author has proved the following theorem:

Theorem 1 (Learning to predict ground state representations; informal). *For any smooth family of Hamiltonians $\{H(x) : x \in [-1, 1]^m\}$ in a finite spatial dimension with a constant spectral gap, the classical machine learning algorithm can learn to predict a classical representation of the ground state $\rho(x)$ of $H(x)$ that approximates few-body reduced density matrices up to a constant error ϵ when averaged over x. The required training data size N and computation time are polynomial in m and linear in the system size x.*

The author used the classical shadow representation of a quantum system to be the training and testing data, i.e., given x (will be m parameters), the model predicts the classical representation.

In 3.2, we demonstrate another situation. Given now x to be the parameters of a quantum circuit, we would like to see whether classical machine learning model can learn the quantum circuit. The motivation is to see whether classical machine model are able to learn the quantum machine learning model. Also, the classical shadow representation can be used on a quantum circuit. We will demonstrate with the simplest ansatz - variational quantum circuit with single qubit rotation gates. The ansatz will be built in the following way:

(i):Construct a quantum circuit with n-qubit.

(ii):We apply a 3-parameter single qubit rotation gate on each qubit, each with different parameters. Then we apply a sequence of **CNOT** gates on each two adjacent qubits (including the first and the last qubit).

(iii):We repeat step.(ii) with l times, corresponding to l layers.

3 Result and Analysis

The code will be available at

3.1 Test the performance of Classical Shadow Representation

In this subsection, we demonstrate the performance of classical shadow representation in different configuration setup of quantum system. We simulate a quantum system as discussed in 2.3, the configuration hyper-parameters we used are given in table 3.1. An example of a quantum circuit ansatz is given in figure 3.1.

Table 1: Configuration of simulated quantum system with quantum circuit

number of qubits	2,3,4,5
number of layers	1,2
number of shots	1E2, 1E3, 1E4, 1E5
random seeds	25 different seeds

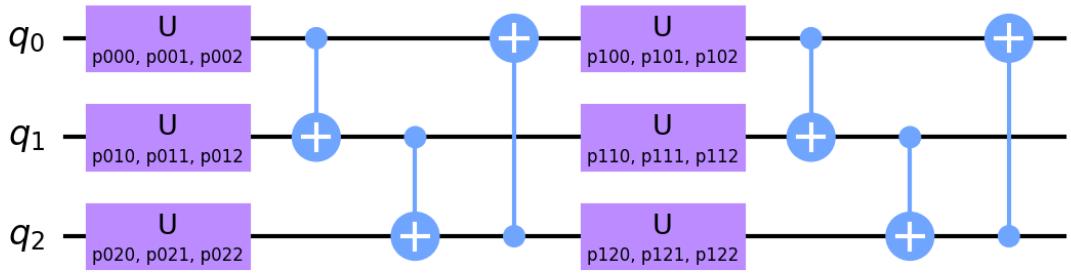

Figure 1: Example of quantum circuit ansatz with 2 layers and 3 qubits.

In each configuration setup, we calculate the Hilbert-Schmidt and Frobenius norm discussed in 2.2. To see the performance of classical shadow representation, we choose the compared reference to be another randomly generate classical shadow representation. The only difference is that the σ_i' are now generated by purely random, instead of randomly measured from the quantum system. That is, consider σ_T'

$$\sigma_T' = \frac{1}{T}\sum_{t=1}^{T} \sigma_1'^{(t)} \otimes \sigma_1'^{(t)} \otimes ... \otimes \sigma_n'^{(t)} \quad \text{where} \quad \sigma_i'^{(t)} = 3\left|r_i^{(t)}\right\rangle\left\langle r_i^{(t)}\right| - \mathbb{I} \tag{2}$$

the $\left|r_i^{(t)}\right\rangle$ are now just a randomly selected basis, not from measurement outcome. The comparison result is in figure 3.1. As expected, the Hilbert-Schmidt inner product of classical shadow representation should be higher than randomly generated density matrix. Also, the tendency of Frobenius norm get lower when the number of shots (corresponding to T copies) increases. However, it is unclear why the randomly generated density matrix is not constant in Frobenius case, also, the random generated density matrix has less Frobenius norm than expected. (Note that we calculate the Frobenius norm of the difference to true density matrix.)

3.2 Predicting Classical Shadow Representation of a given quantum circuit

In this subsection, we demonstrate learning a quantum model with the ansatz given in 2.3. The quantum model can be thought as a trained variational quantum circuit. We then feed some x into the quantum circuit and get the classical shadow representation, different x can be thought as different parameters in a Hamiltonian. The main goal is to train a classical machine learning model to learn to predict the classical shadow representation of the quantum model. The detail of training is given in the following steps:

(i) Create training and testing data with the rotation gate ansatz 2.3. We will use $T = 100$ copies for every different parameter x to get their classical shadow representation. We also get their exact density matrix. The classical shadow representation will be used for training, since it mimics the real experiment data. The exact density matrix only used for discussing the performance of training with classical shadow representation.

(ii) Build up a classical machine learning model with fully connected linear layers and activation functions ReLU. The input will be x, and the output will be a "modified" classical shadow representation. The output dimension will be $s * q * 6$ where s stands for the number of copies we want, q is the number of qubit, and 6 stands for the number of 6 basis. The final layer of the classical model will be a softmax over each 6 basis. Then the final output will be a "superposed" classical shadow, that is, if the output value can be labeled as $C_{q,i}^{(s)}$ where i is from 1 to 6, the predicted

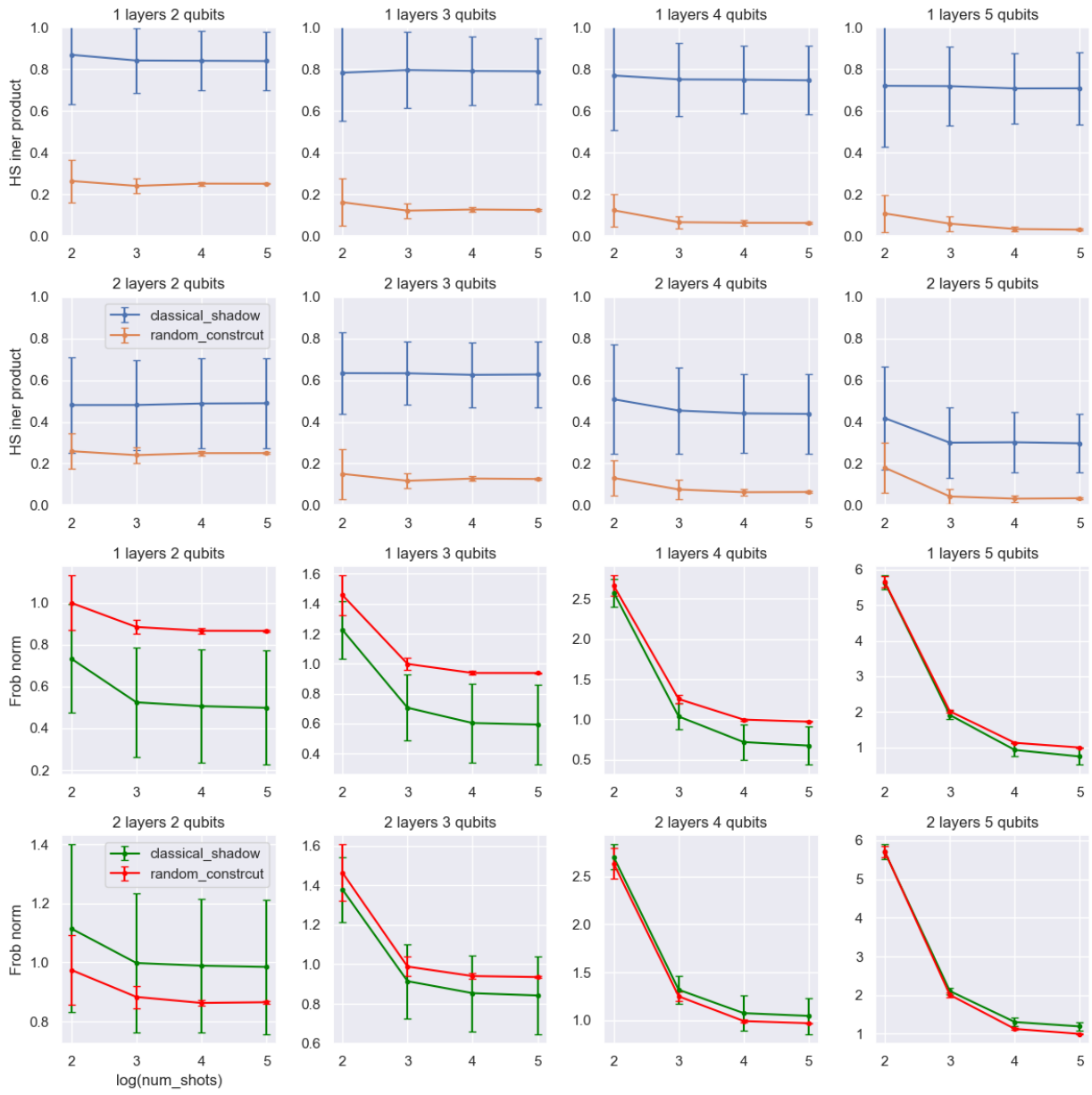

Figure 2: Result of comparison. The first two rows and the last two rows are compared with Hilbert-Schmidt inner product and Frobenius norm respectively. Each figure is calculated with different number of qubits and number of layers.

classical shadow will be

$$\hat{\sigma}_{\text{predict}} = \frac{1}{s}\sum_{t=1}^{s}[(\sum_{i=1}^{6} C_{1,i}^{(t)}\sigma_i^{(t)}) \otimes ... \otimes (\sum_{i=1}^{6} C_{q,i}^{(t)}\sigma_i^{(t)})] \tag{3}$$

The σ on the RHS is similar as defined in equation 2, but with the all 6 basis considered. Notice that the trace of $\hat{\sigma}$ is still 1.

(iii) We will set the cost function to be the negative of Hilbert-Schmidt inner product with the classical shadow representation generated in step (i). The physical meaning is to let the trained $\hat{\sigma}$ to be as close to the classical shadow data in the aspect of Hilbert-Schmidt inner product.

(iv) We will also test the $\hat{\sigma}$ we trained in every epoch and the true classical shadow representation with random measurement. That is, we will randomly measure each qubit in X, Y or Z basis, then compare their expectation value. We will record the absolute difference, as will be seen in the figure 3.2 (the red lines).

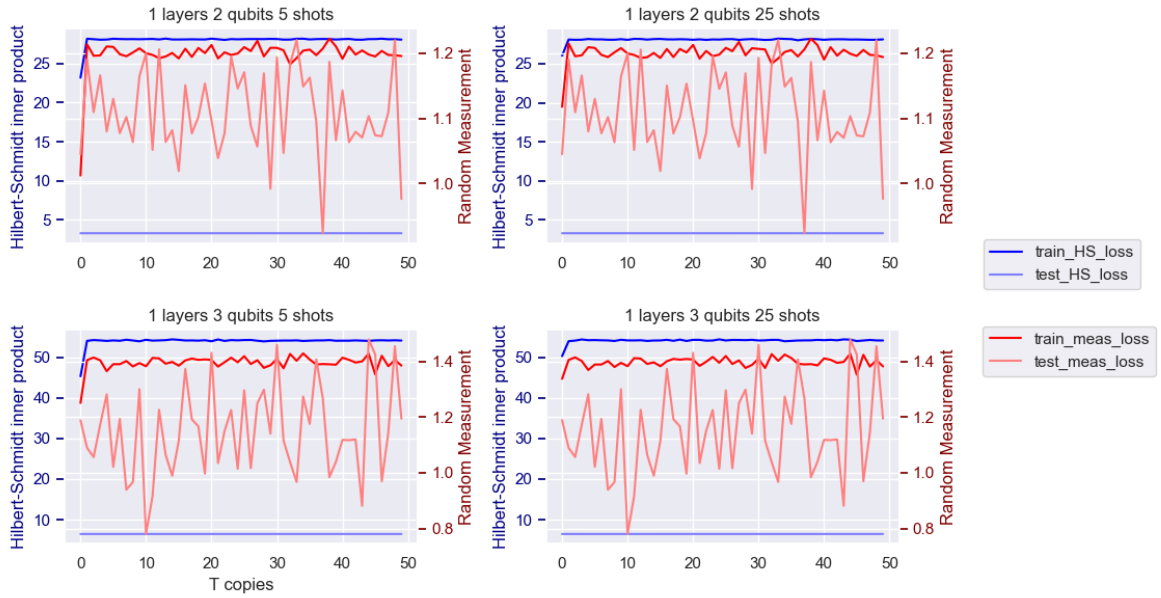

Figure 3: Result of machine learning to predict the classical shadow representation. The blue colors are the training and testing result of Hilbert-Schmidt inner product. The red colors are the training and testing result of difference of expectation values of random measurements.

The result of training is not quite satisfying, seems like the model might be over-training, since the Hilbert-Schmidt inner product has successfully decrease. Something remains unclear is that both the results of random measurement are not decreasing, but we should expect it should decrease as the Hilbert-Schmidt inner product increase. Due to the limitation of computation resource, we guess the result should be as we expected after fine tuned or try other model structure.

4 Discussion and Conclusion

Classical shadow representation gives people a more efficient way to store the information of data coming out of a quantum system. The power of classical shadow representation has been shown in some papers [1] [2] [3]. Also, when we code with an open source *pennylane*, the classical shadow method is also included in there packages. We are looking forward for the applications of classical shadow representation. Last but not the least, we are really appreciate for the nice talk from Robert Huang, and also the work from him.

All of the source code written by us can be found at `https://github.com/r08222011/Quantum_Classical_Shadow_ML`.

References

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