Quantum Neural Networks for Analyzing X-Ray Scattering Data

Vinit Kumar Singh
Department of Physics
Indian Institute of Technology
Kharagpur, WB 721302, India
vinitksingh@iitkgp.ac.in

Brenda Rubenstein †
Department of Chemistry
Brown University
Providence, Rhode Island 02912, USA
brendarubenstein@brown.edu

***Abstract*—Determining the chemical structures of molecules from scattering cross-section has been a long-standing problem in chemistry. To date, it is accomplished by performing massive molecular dynamics simulations. To avoid such calculations researchers have developed Classical Machine Learning (CML) methods. But the sheer complexity of the problem requires vast Neural Networks and enormous datasets. Quantum Machine Learning (QML) on NISQ computer has shown great potential in dealing with such problems with exponentially smaller resources. Here we demonstrate the operation of simple Quantum Neural Network (QNN) architectures that can provide insights in the dataset by using just a few qubits and small sample sizes. We explore various parameterized quantum circuits, state preparation schemes, and circuit decomposition algorithms. Finally, we present a comparison between the QML and CML approach.**

POSTER RELEVANCE

By efficiently predicting the molecular structures from the X-ray scattering data using Quantum Neural Networks, we can reveal fundamental principles of molecular reactions. Quantum Machine Learning promises to become an area of extraordinary technological importance as practical quantum computers become more prevalent in the coming decades. The work we propose will be a significant contribution towards the ultimate goal of data classification using high-level features. The results demonstrate the advantages of quantum computing and machine learning in discoveries of rare signals or trends in massive data. It may provide insight on if, and how, the parallel execution of multiple processes using qubits may be able to speed up certain types of problems effectively. The implications of the speed up are rather significant for X-ray scattering experiments in which the complexity of the data will be unprecedented and the current techniques will certainly fail; thus, alternative strategies are needed.

POSTER: EXTENDED ABSTRACT

A. Introduction

The advent of ultrafast-pulsed X-ray free electron lasers (XFELs) and mega-electron-volt electron sources can lead to a paradigm shift in chemistry. XFELs, such as Linac Coherent Light Source (LCLS), provide short duration X-ray pulses that enable chemists to be able to follow the time course of the structural and electronic changes that molecules undergo with ¡100 fs and 10 mÅ resolution. The researchers of [1] uses this world-class equipment to image the complicated ring-opening reaction of 1,3-cyclohexadiene (CHD) and vibrational relaxation of hot N-methylmorphonline. But, these experiments produce a deluge of X-ray scattering data that must be analyzed and matched to known chemical structures. Typically data sets consists of millions of X-ray shots weighing about 10-100s of TBs. To date, this analysis is accomplished with Molecular dynamics simulations. These calculations are time-consuming and produce large amounts of redundant information, but they can yield physically questionable structures because accurately modeling quantum dynamics remains one of the longest-standing problems in all of chemical physics.

Quantum Machine Learning (QML) [3], [7], [8] algorithms provide promising solutions to deal with this data deluge while using exponentially smaller resources. The Entanglements among the qubits allows QNN circuit to learn hidden correlations in the dataset. The QML algorithms use quantum circuits which are controlled by parameters and are famously known as Quantum Neural Networks (QNNs). In analogy with classical deep learning, the parameters of a QNN can be optimized with respect to a cost function via gradient-based methods. The availability of Noisy Intermediate-Scale Quantum (NISQ) processors has increased interests in Hybrid Quantum-Classical Machine Learning (HQCML) Algorithms. In HQCML algorithms, the optimization of the parameters of QNN are carried on a classical computer whereas the evaluation of the quantum circuit requires a Quantum Processing Units (QPUs).

B. Computational Details

1) Inputs and Outputs: The problem at hand is to predict the molecular geometry of N-methyl-morpholine (NMM) from its X-ray scattering data. The input data set consists of the scattering cross-section of the NMM molecule for the different geometries contained in the output. The output data consists of the degrees of freedom of all of the non-hydrogen NMM atoms. There are fifteen non-hydrogen atomic degrees of freedom, out of which the first six are bond lengths, the second five are adjacent atom bond angles, and the last four are dihedral angles. These are obtained from the z-matrix representation of the molecule. To enhance the performance of the ML algorithms we perform a Principal Component

Analysis (PCA) on the input data and consider only first 20 principal components.

2) State Preparation: The QML algorithms primarily depend on encoding of the classical data stored in classical bits into qubits. In our work we perform the quantum state preparation using Amplitude Encoding scheme. In this scheme an $O(n)$-dimensional classical vector is encoded into $O(\log n)$ qubits. $\vec{x} \equiv (x_0, x_1, x_2, ...x_n) \longrightarrow |x\rangle = \sum_{i=1}^{\log n} x_i|i\rangle$ where $|x\rangle$ is the final quantum state and the $|i\rangle$'s are the computational basis vectors. Before starting the encoding process the classical input data is normalized because they have to represent the amplitudes of a quantum state which has a unit norm. The paper [4] describes how Amplitude encoding is performed.

3) Circuit Decomposition: A quantum computation corresponds to a unitary operation, and a universal quantum computer should be able to perform arbitrary unitary operations with very high precision. In practise it is efficient to break down huge multi-qubit unitary operations into simpler gates. The paper [5] describes a formalism to perform Circuit Decomposition of Arbitrary Unitary Gates using just single-qubit rotation gates and CNOT gates. In our work we use Cosine-Sine Decomposition mentioned in Section IV D of [5].

4) Quantum Neural Network: Since we are working with relatively small number of qubits, we use a Parameterized n-qubit Unitary Rotation Gate as the Quantum Neural Network. A universal n-Qubit Unitary Rotation Gate can be constructed using only $n(n-1)$ Single-Qubit Rotation Gates and $n(n+1)$ CNOT Gates as show in [6]. As every Single-Qubit Rotation Gate can be completely represented using three variables, the whole n-Qubit Gate has $3n(n+1)+n(n-1)$ parameters, where each CNOT has a parameters indicating if it is activated or deactivated. The QNN is fed with 2^n-dimensional classical input feature vector encoded into n-qubits. The State Preparation is followed by a $(n+1)$-qubit Parameterized Quantum Circuit. Finally the last ancilla qubit is measured to retrieve a classical output.

5) Classical Optimization: After the measurement of the output quantum state from the quantum neural network, the information is classical again and we can make use of classical computers to perform optimization. The process exactly same as in CML. First there is computation of cost function and then their is gradient descent over the free parameters. There are various algorithms developed to compute the gradients of Quantum Neural Network. The Section V of [9] investigated Quantum Stochastic Gradient Descent for Mean Square Error (MSE).

C. Results

1) Testing QNN on Quantum Fourier Transform (QFT): : We got a nearly perfect accuracy while predicting QFT, which is not surprising because ultimately QFT is a subset of Unitary transformation on n-qubits.

2) Comparison between Classical and Quantum Neural Networks: We used the standard Fully-Connected layered Classical NN to demonstrate the comparison. The network contained three layers containing 475 perceptrons each. The activation function of choice is Rectified Linear Unit (ReLU). The comparison between QNN and Classical NN isn't fair for a number of reasons. The sample size of QNN (Classical NN) is 1000 (1 million), it has 168 (around 470,000) trainable parameters, the learning rate is 0.01 (1e-4), and the number of epochs is 8 (50). These limitations on QNN arise from its slow operation and limited number of qubits accessible. To make the comparison fair we trained another smaller Classical neural network with sample size of 1000, 6915 learnable parameters (only 50 perceptrons in each layer), learning rate of 1e-4 and 200 epochs. The results are summarized in the poster. It is interesting to see that our QML algorithm learns insights in the dataset even with so few qubits and a small dataset.

D. Discussion

While the use of classical processors as outer-loop optimizer for HQCML is promising, the reality is that near-term quantum devices are still fairly noisy, thus limiting the depth of quantum circuit achievable with acceptable fidelity. Moreover, the QML algorithms are dependent on fast quantum state preparation techniques that can encode classical data into qubits to achieve quantum speedups. Without the invention of Quantum RAMs, the state preparation can be extremely time consuming and could possibly lead to the loss of speed-up that quantum computers promise to offers. QML algorithms also suffers from issues relating to vanishing gradient. This is a common problem in both QML and CML. There is a theorem that states that random initialisation of Quantum Gate parameters leads to quick decay of gradient called the Barren Plateau problem. The problem can be fixed by following a protocol called Identity Block Initialisation.

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