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Application of Quantum Machine Learning to High Energy Physics Analysis at LHC using IBM Quantum Computer Simulators and IBM Quantum Computer Hardware

J. Chan[a], W. Guan[a], S. J. Sun[a], A. Wang[a], S. L. Wu[a], C. Zhou[*a], M. Livny[b], F. Carminati[c], A. D. Meglio[c]

[a]*Physics Department of University of Wisconsin-Madison, US*[†]
[b]*Computer Sciences Department of University of Wisconsin-Madison, US*
[c]*CERN openlab, IT Department, CERN, CH*
E-mail: chen.zhou@cern.ch

The ambitious HL-LHC program will require enormous computing resources in the next two decades. A burning question is whether quantum computer can solve the ever growing demand of computing resources in High Energy Physics in general and physics at LHC in particular.Using IBM Quantum Computer Simulators and Quantum Computer Hardware, we have successfully employed the Quantum Support Vector Machine Method (QSVM) in applying quantum machine learning for a ttH (H to two photons), Higgs coupling to top quarks analysis at LHC.

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1. Introduction

The ambitious HL-LHC program will require enormous computing resources in the next two decades and beyond. New technologies are being sought after to replace the present computing infrastructure. A burning question is whether quantum computer can solve the ever growing demand of computing resources in High Energy Physics in general and physics at LHC in particular. Our goal here is to explore and to demonstrate that Quantum Computing can be the new paradigm (Proof of Principle).

The experimental programs of LHC revolve around one major objective: discovery of new physics. This requires the identification of rare signals against immense backgrounds. Using machine learning algorithms greatly enhance our ability to achieve this objective. The authors in this paper are from one of the LHC groups which has pioneered the use of machine learning in high profile physics analysis. We have used machine learning algorithm on the measurement by the ATLAS Collaboration of Higgs coupling to top quark pairs (ttH). The impact of this ttH channel resulted in the CERN press release on June 4, 2018 [1, 2]. However, with a fast increasing volume of data in the future HL-LHC program, applying quantum machine learning method may well be a new direction to go.

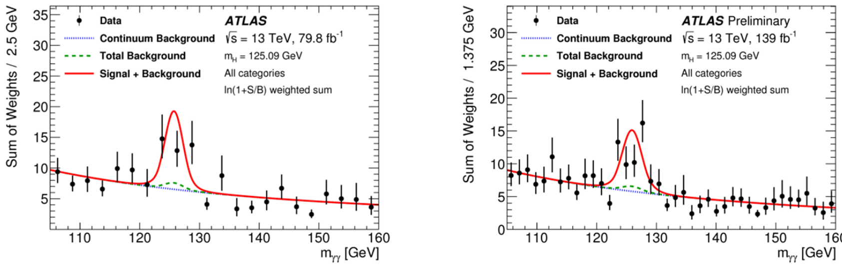
In this paper, we have shown good progress in the LHC physics channel ttH (Higgs coupling to the top quark) with quantum machine learning algorithms using IBM Quantum Simulator and IBM Quantum Computer Hardware.

2. ttH (Higgs coupling to the top quark) at LHC

As only 1% of all Higgs bosons are produced in association with top quarks, its observation [1, 2] was extremely challenging. Since the discovery of the Higgs boson in 2012, this is one of the physics processes focused at LHC. We address here the channel where the Higgs decays into two photons. In the ATLAS Collaboration, analysis optimization employing advanced machine learning techniques to obtain the best sensitivity in the measurement of the ttH (H to 2 photons) process was successful. The XGBoost package [3], which is currently one of the most advanced Boosted Decision Tree (BDT) algorithms available, is utilized in this analysis. Both ttH simulation and data control region samples are separated into three non-overlapping parts, for BDT training, hyper-parameter tuning, and sensitivity evaluation, respectively. The BDT training uses kinematic variables (four vectors) of jets, leptons, and photons, to maximize the usage of event information and thus separate the ttH signal from the major backgrounds. Furthermore, to exploit the BDT separation power, multiple event categories with different BDT score ranges are defined. A simultaneous diphoton mass fit over all the event categories is then performed to extract the ttH signal strength.

In this channel alone, with ATLAS data, the ATLAS Collaboration has observed a significance of 4.1 standard deviations with 80 fb^{-1} of 2015-2017 data. In combination with other channels, the ATLAS Collaboration achieved a significance of 6.3 standard deviations. Thanks to the analysis optimization based on machine learning techniques, the current ttH (H to 2 photons) analysis is 50%-60% more sensitive than the previous result [5]. This improvement in sensitivity was the key to the ttH process observation by the ATLAS Collaboration. In summer 2018, the ATLAS

PoS(EPS-HEP2019)116



(a) (b)

Figure 1: The mass spectra of two photons in the ttH (H→2 photons) analysis by the ATLAS Collaboration, with (a) 80 fb^{-1} and (b) 139 fb^{-1} of data [1, 4]. These spectra peak at the Higgs mass of 125 GeV. They give a strong evidence of the Higgs production in association with two top quarks. While classical BDTs are utilized in this analysis, it is our goal here to improve this analysis with a Quantum Machine Learning platform.

and CMS Collaborations at CERN announced the observation of Higgs bosons produced together with a top-quark pair (ttH) with a CERN press release and publications [1, 2]. Observing this extremely rare process is a significant milestone for the field of High-Energy Physics related to the Higgs Boson. It confirms the Yukawa interactions between the Higgs boson and the top quark, which is the heaviest known elementary particle, with the predicted strength. Recently, with 139 fb^{-1} of data (including data collected in 2018) and with the ttH (H to 2 photons) channel alone, a significance of 4.9 standard deviations was observed, up from 4.1 standard deviations in 2018. This is the first observation in a single channel of the ttH process, and the result has been released by the ATLAS Collaboration at the Moriond 2019 conference [4].

The mass spectra of two photons in the ttH (H to 2 photons) analysis by the ATLAS Collaboration is given in Figure 1, with 80 fb^{-1} (a) and 139 fb^{-1} (b) of data [1, 4]. These spectra peak at the Higgs mass of 125 GeV. They give a strong evidence of the Higgs production in association with two top quarks.

3. Quantum Machine Learning Algorithm: Quantum Support Vector (QSVM)

The intersection between machine learning and quantum computing has been referred to as Quantum Machine Learning. With the progress of quantum technologies, the application of Quantum Machine Learning emerges as a possible powerful tool for data analysis in HEP in the future. The QSVM is the method we have used in our work in progress. It includes the QSVM Kernel method and the QSVM Variational method. A Support Vector Machine (SVM) is a supervised machine learning method in which a hyperplane is constructed to separate labeled samples between two classes of data points. With the emergence of quantum technologies, a Quantum Support Vector Machine (QSVM) kernel method [7] was developed with mapping input vectors to a Hilbert space. In 2018, a variational QSVM method [6] was introduced by Gambetta and coworkers published in NATURE with a quantum circuit implementation. In this publication [6], the IBM scientists implemented both QSVM Kernel and QSVM Variational methods extensively. Following [6] we propose to look for new mapping of the classical SVM approach into a quantum algorithm in

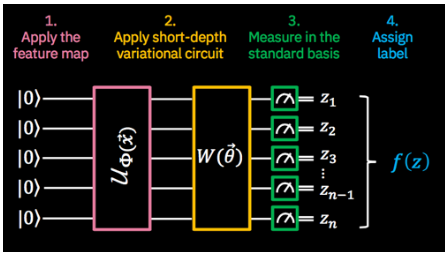


Figure 2: Sketch of the variational quantum SVM algorithm with its steps: 1. Loading of the data by means of the feature map; 2. Application of the variational circuit; 3. Read out of the final qubit state, and 4. Assignment to the different classes [6].

which the feature map is evaluated in the Hilbert space of the N-qubit system. The variational QSVM approach is summarized in four main steps as shown in Figure 2, which is taken from the supplementary information to [6].

4. Applying Quantum Machine Learning to ttH analysis

Although the era of efficient Quantum Computing may still be some years away, we have made promising progress and obtained preliminary results in the application of IBM Quantum Computer Simulators and Quantum Computer Hardware to LHC ttH data analysis. The workflow is shown in Figure 3. All events used in this paper are simulated with Delphes [8]. In the present work, each variable of an input event is encoded in the amplitude of one separate qubit. However, we have many more variables per event than available qubits. Therefore, we employed Principal Component Analysis (PCA) to reduce input events to fewer variables to match the available number of qubits. In a next step in the future, we would like to enhance the quantum feature map method (encoding classical variables to quantum states) to encode as many variables as possible with limited qubits in order to remove the PCA step.

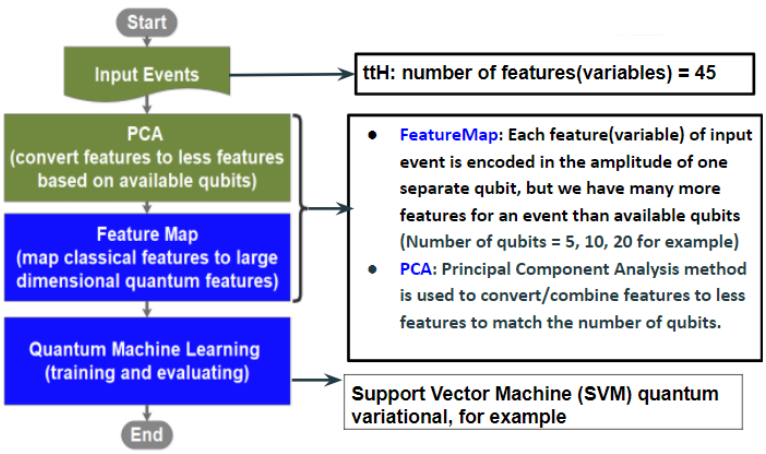


Figure 3: Quantum Machine Learning Workflow.

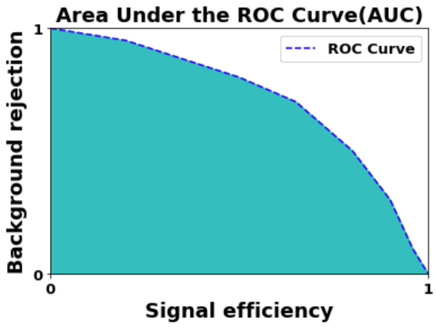


Figure 4: Definition of AUC (Area Under Curve) and ROC (Receiver Operating Characteristics) Curve.

The results can be summarized as follows:

(a) Employing QSVM Variational Method with IBM Quantum Computer Simulators Using IBM Quantum Computer Simulators, we have successfully employed the Quantum Support Vector Machine (QSVM) for ttH (H to two photons), Higgs coupling to top quarks analysis at the LHC. We have measured the AUC (area under the ROC curve) with different numbers of events. Here the ROC curve is defined as the Receiver Operating Characteristics curve in the plane of background rejection versus signal efficiency - see Figure 4. At our current stage, with 5 qubits and 800 events we have reached an AUC of 0.86, which is close to the AUC of 0.87 from a Classical Machine Learning method (BDT), with the same input. It is however still far from the LHC analysis with all 45 variables and thousands of events, as shown in Figure 5 (black curve).

We also perform a preliminary study applying the quantum SVM machine learning algorithm to the Higgs to two muons analysis with Delphes simulation events using the IBM quantum computer simulators.

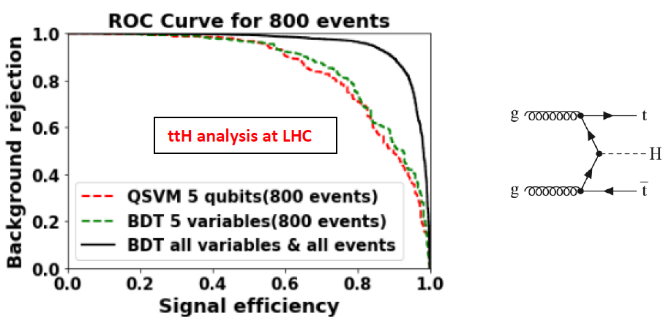


Figure 5: The ROC Curve plot of QSVM (red) with 5 qubits and BDT (green) with 5 variables for 800 events, and the ROC Curve (black) of the Classical Machine Learning BDT for all 45 variables and thousands simulated events in ttH analysis. With limited qubits and limited numbers of events, QSVM (red) reached a similar performance as BDT (green). However it is still far from LHC analysis with all variables and all events (black curve). One of our goal is to scale up our analysis to all variables and all events. The Feynman diagram for the ttH process is shown on the right.

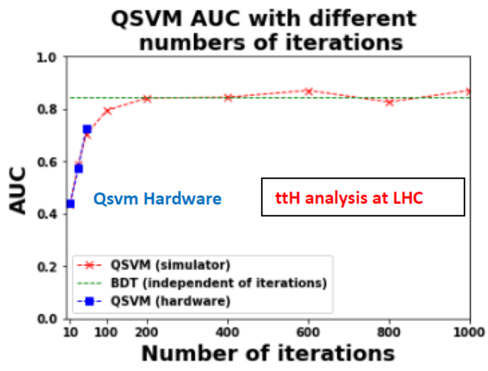


Figure 6: QSVM Variational Method with IBM Quantum Simulators and IBM Quantum Computer Hardware: the AUC with different numbers of computing iterations. With limited test iterations, QSVM on hardware (blue square) gives results compatible with those from Quantum Computer Simulators (red). Here another one of our goals is to scale up our analysis on Quantum Computer Hardware with enough iterations.

(b) Employing QSVM Variational Method on IBM Quantum Computer Hardware

- Collaborating with IBM Research, Zurich, we performed training with machine learning on the IBM Quantum Computer Hardware with 100 training events, 100 test events, and 5 qubits, again for the ttH (H to two photons) analysis at the LHC. Because of hardware access time and timeout limitations, we only finished a few iterations (for example 10, 30, 50) on the hardware, compared to several thousand iterations on the simulators. The limitation of access time for 5 qubits or higher (10, 20 qubits) will be alleviated in our future collaboration with IBM.
- As shown in Figure 6, with limited iterations, the result from hardware (blue square) is compatible with the result from the Quantum Simulator (red) in tested iterations. The result from the Quantum Simulator (red) reached a similar performance to that of the classical BDT method (green) with enough iterations.

5. Summary

The era of efficient Quantum Computing may still be some years away. We have made promising progress and obtained preliminary results in the application of Quantum Support Vector Machine on IBM Quantum Simulators and IBM Quantum Hardware. We are extending our analysis to more physics variables and larger number of events with limited number of qubits and we will enhance the performance. Furthermore, since quantum hardware is still in its intensive stage of development, we need to work out a more effective way in applying quantum simulators to our high energy physics application, given the importance of simulation power in this early work before we have large scale quantum hardware.

6. Acknowledgement

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PoS(EPS-HEP2019)116