Application of Quantum Machine Learning in some LHC and CEPC Data Analyses

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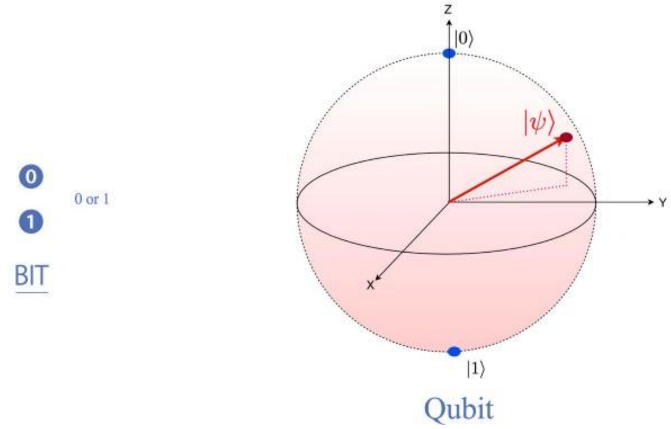
Disclaimer: I am not an expert of quantum machine learning.
Today I will focus on the quantum machine learning applications that I have been studying within two collaborations.

Machine learning for High Energy Physics

- One of the major objectives of the experimental programs at the LHC is the discovery of new physics.
- Machine Learning: “application of artificial intelligence that provides systems the ability to automatically learn and improve from experience without being explicitly programmed”
  - It has become one of the most popular and powerful techniques and tools for High Energy Physics (HEP) data analysis
  - It greatly enhances our ability to identify rare signal against immense backgrounds: important for discovery of new physics
- Issues raised by machine learning
  - Heavy CPU time is needed to train complex models
    - The training time increases with more data
  - May lead to local optimization, instead of global optimization

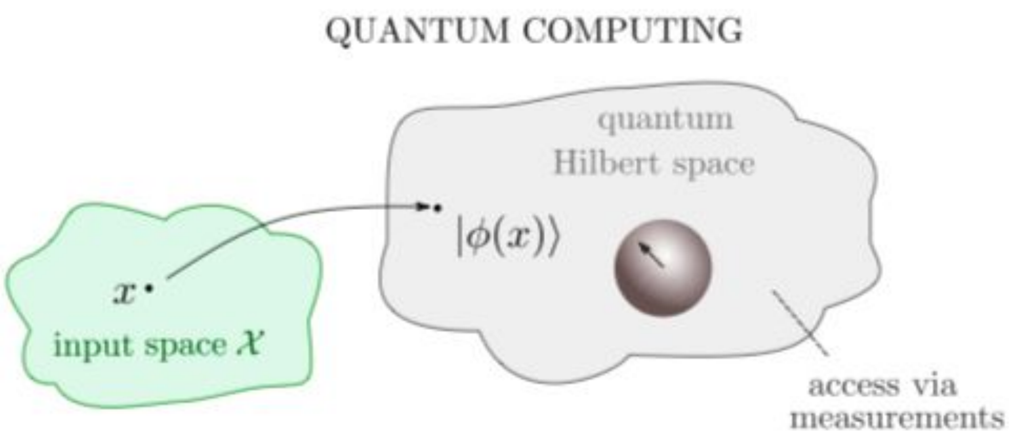
Quantum Machine learning

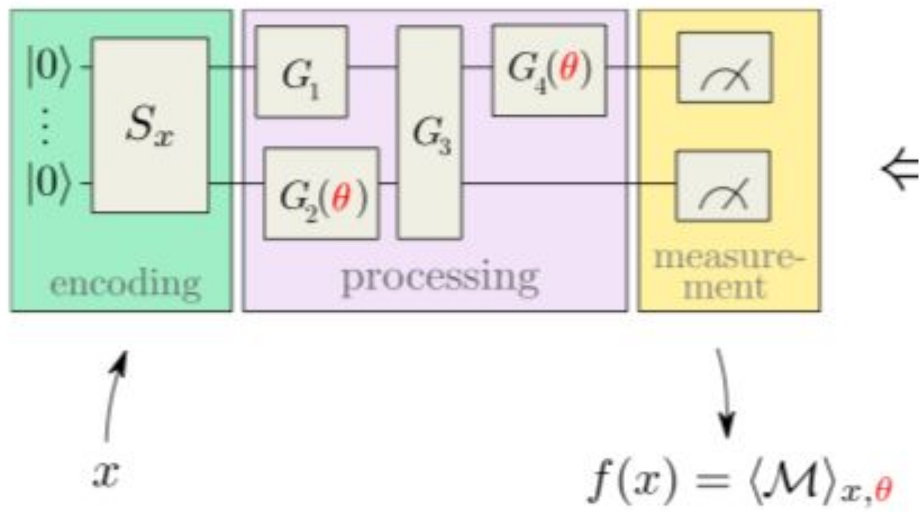


- Quantum computing
  - Perform computation using the quantum state of qubits
  - A way of parallel execution of multiple processes
  - Can speed up certain types of problems effectively
- Quantum machine learning
  - Intersection between machine learning and quantum computing
  - May lead to more powerful solutions and offer a computational "speed up", by exploiting the high dimensional quantum state space through the action of superposition, entanglement, etc
  - Quantum machine learning could possibly become a valuable alternative to classical machine learning for HEP data analysis

Quantum Machine learning

- **Quantum machine learning algorithms encode input data to a quantum state, "process" (transform) the quantum state, and access the quantum state via measurements**





Maria Schuld [*arXiv:2101.11020*]

Quantum Machine Learning application for HEP

- Maria Spiropulu et al, “Solving a Higgs optimization problem with quantum annealing for machine learning”, Nature 550, 375 (2017)
- …
- Plus many more on Monte Carlo generation/simulation, particle reconstruction and physics data analysis using gate-model quantum computers, quantum annealers, and photonic quantum computers

Our Goal:

To perform High Energy Physics analysis with Quantum Machine Learning, to explore and to demonstrate that the potential of quantum computers can be a new computational paradigm for big data analysis in HEP, as a proof of principle

Example 1

Employing Variational Quantum Classifier for ttH (H $\rightarrow \gamma\gamma$) and H $\rightarrow \mu\mu$ analyses

J. Phys. G: Nucl. Part. Phys. 48 125003 (2021)

I was in an international and interdisciplinary team of High Energy Physicists and Quantum Computing Scientists assembled by Prof. Sau Lan Wu (University of Wisconsin):

Jay Chan, Alkaid Cheng, Wen Guan, Shaojun Sun, Alex Wang, Sau Lan Wu, Rui Zhang, Chen Zhou

Physics Department, University of Wisconsin-Madison

Miron Livny

Computer Sciences Department, University of Wisconsin-Madison

Federico Carminati, Alberto Di Meglio

CERN Quantum Technology Initiative, IT Department, CERN

Panagiotis Barkoutsos, Ivano Tavernelli, Stefan Woerner, Jennifer Glick

IBM Research Zurich and IBM T.J. Watson Research Center

Andy Li, Joseph Lykken, Panagiotis Spentzouris

Quantum Institute, Fermilab

Samuel Yen-Chi Chen, Shinjae Yoo

Computational Science Initiative, BNL

Tzu-Chieh Wei

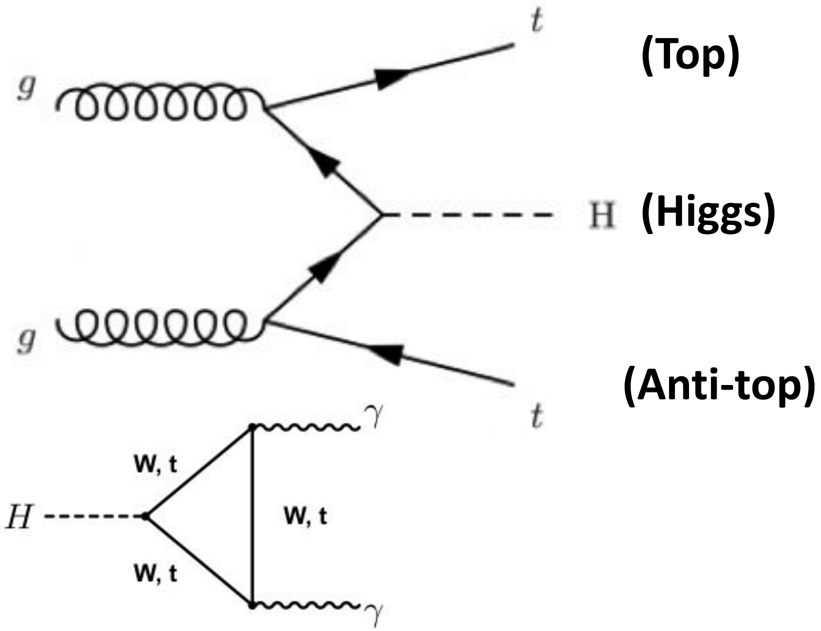
C.N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook

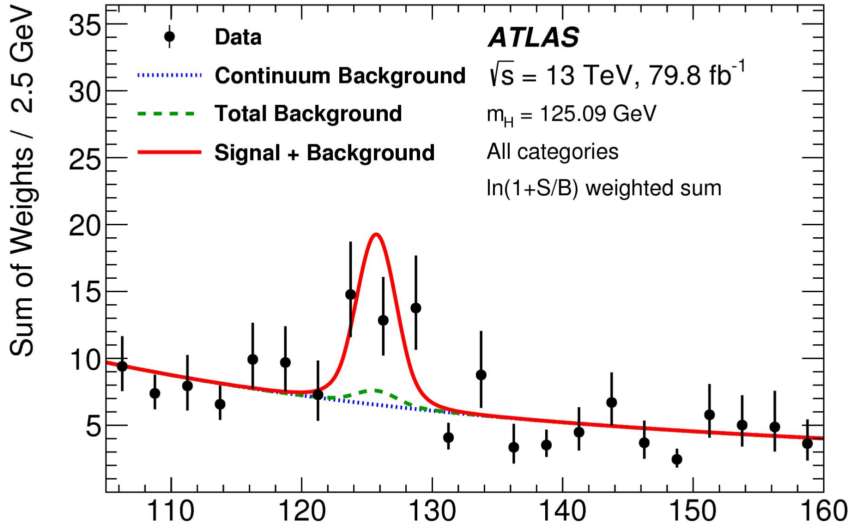
Pavel Lougovski, Sanjay Padhi, Simone Severini, Dewayne Walker

Quantum Computing and AI Research, Amazon Web Services

ttH (H → γγ) analysis at the LHC

The observation of ttH production (Higgs boson production in association with a top quark pair) by ATLAS and CMS at the LHC directly confirmed the interaction between the Higgs boson and the top quark, which is the heaviest known fundamental particle



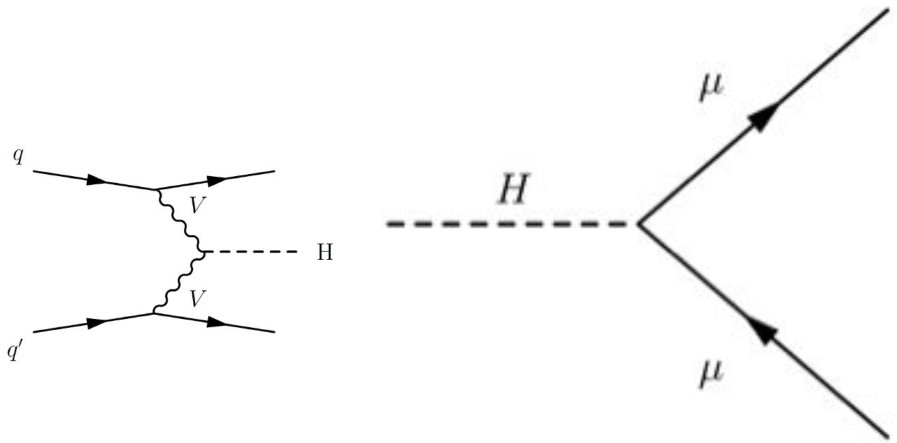


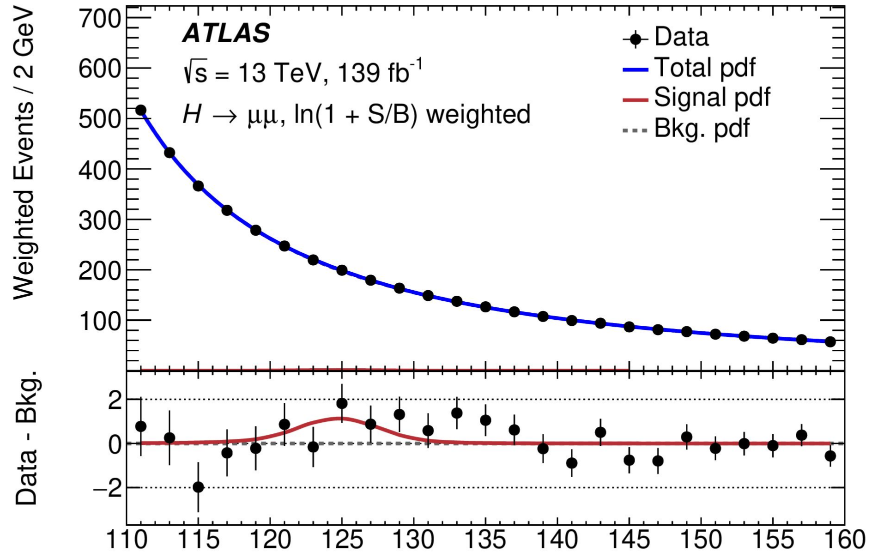
[Phys. Lett. B 784 (2018) 173] $M_{\gamma\gamma}$ [GeV]

- **Using Boosted Decision Tree (BDT, a classical machine learning technique) with XGBoost package, the ATLAS Collaboration observes the ttH (H→γγ) process**
- **Our study performs the event classification of the ttH (H→γγ) analysis (hadronic channel) with delphes simulation samples and quantum machine learning**

H → $\mu\mu$ analysis at the LHC

Although the coupling between the Higgs boson and 3rd-generation fermions has been observed, currently the coupling between the Higgs boson and 2nd-generation fermions is under intensive investigation. H→$\mu\mu$ is the most promising process to observe such a coupling by ATLAS and CMS at the LHC





[Phys. Lett. B 812 (2021) 135980](#) **Mμμ [GeV]**

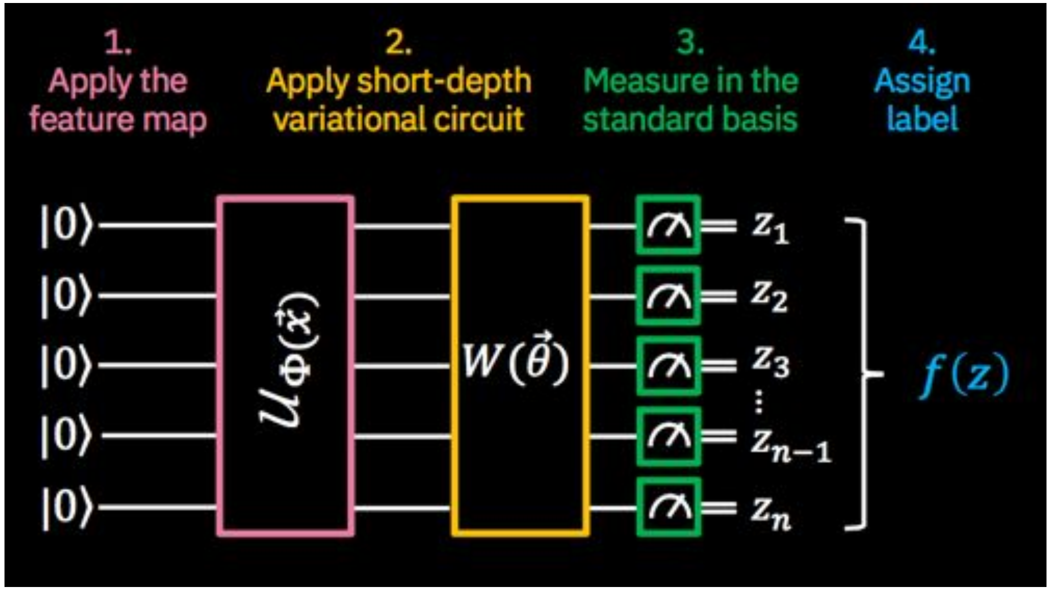
- **Using Boosted Decision Tree (BDT, a classical machine learning technique) with XGBoost package, the ATLAS Collaboration searches for the H→$\mu\mu$ decay**
- **Our study performs the event classification of the H→$\mu\mu$ analysis (VBF channel) with delphes simulation samples and quantum machine learning**

Method 1: Variational Quantum Classifier (VQC)

- **In 2018, a Variational Quantum Classifier method was introduced by IBM, published in Nature 567 (2019) 209.**
- **The Variational Quantum Classifier method can be summarized in four steps.**

Method 1: Variational Quantum Classifier (VQC)

- **1. Apply feature map circuit $U_{\Phi(\vec{x})}$ to encode input data $\vec{x}$ into quantum state $|\Phi(\vec{x})\rangle$**
- **2. Apply short-depth quantum variational circuit W(θ) which is parameterized by gate angles θ**
- **3. Measure the qubit state in the standard basis (standard basis: $|0\rangle$, $|1\rangle$ for 1 qubit; $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$ for 2 qubits; ...)**
- **4. Assign the label ("signal" or "background") to the event through the action of a diagonal operator f in the standard basis**



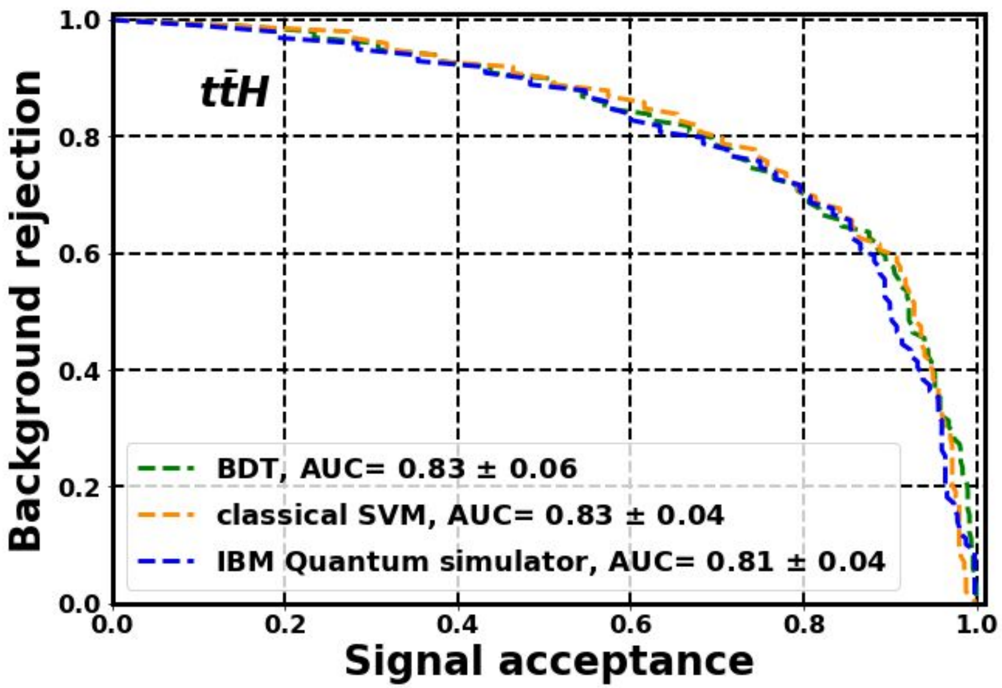
- **During the training phase, a set of events are used to train the circuit W(θ) to reproduce correct classification**
- **Using the optimized W(θ), the testing events are used for evaluation**

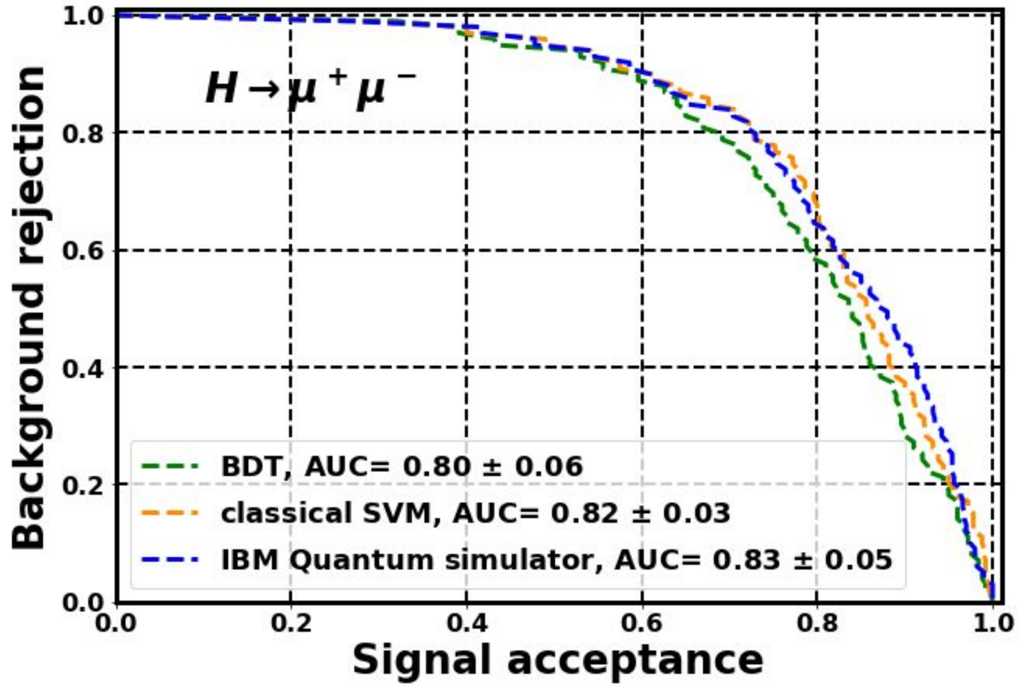
Method 1: Employing VQC (Variational Quantum Classifier) with IBM Q simulator for ttH ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis

Using 10 qubits, we successfully finished training and testing 100 events with IBM Qiskit QASM simulator (where '100' events means 100 training events and 100 testing events).

- **Here IBM Qiskit QASM quantum computer simulator is used. This simulation incorporates the hardware noise**
- **Quantum circuits are optimized to best fit the constraints imposed by hardware (e.g. qubit connectivity, hardware noise) and the nature of data**

Method 1: Employing VQC (Variational Quantum Classifier) with IBM Q simulator for ttH ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis





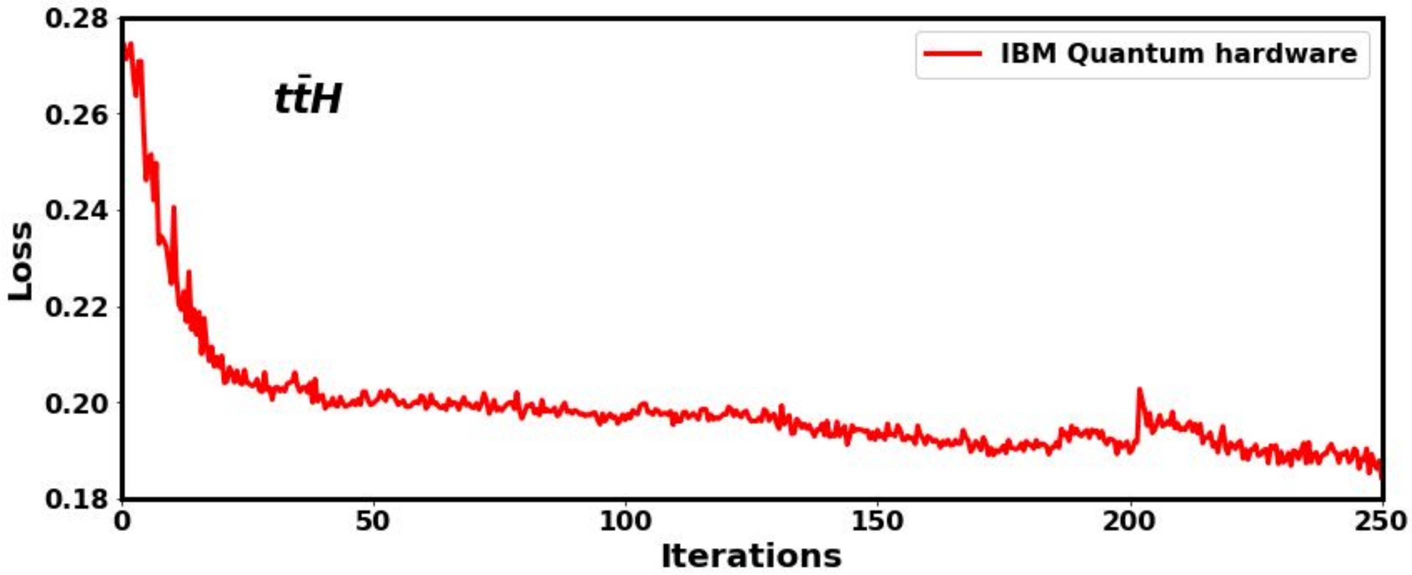
Using ttH analysis dataset (100 events, 10 variables) and $H \rightarrow \mu\mu$ analysis dataset (100 events, 10 variables), Variational Quantum Classifier on simulator (blue) performs similarly with classical BDT (green) and classical SVM (yellow). (Results are average over ten datasets)

	AUC (ttH)	AUC ($H \rightarrow \mu\mu$)
VQC	0.81	0.83
BDT	0.83	0.80
SVM	0.83	0.82

Method 1: Employing VQC (Variational Quantum Classifier) with IBM hardware for ttH ($H \to \gamma\gamma$) analysis and $H \to \mu\mu$ analysis

- **With the help of IBM Research Zurich, Fermilab and BNL, we have carried out a number of jobs on the IBM superconducting quantum computers (ibmq_boeblingen, a 20-qubit machine and ibmq_paris, a 27-qubit machine). In each job, 10 qubits of the quantum computer are used to study 100 training events and 100 testing events.**
  - **The hardware running time for 100 events is 200 hours**
- **For each analysis, due to current limitation of hardware access time, we apply the Variational Quantum Classifier method to one dataset on quantum hardware (rather than ten datasets on quantum simulator)**

Method 1: Employing VQC (Variational Quantum Classifier) with IBM hardware for ttH ($H \to \gamma\gamma$) analysis and $H \to \mu\mu$ analysis



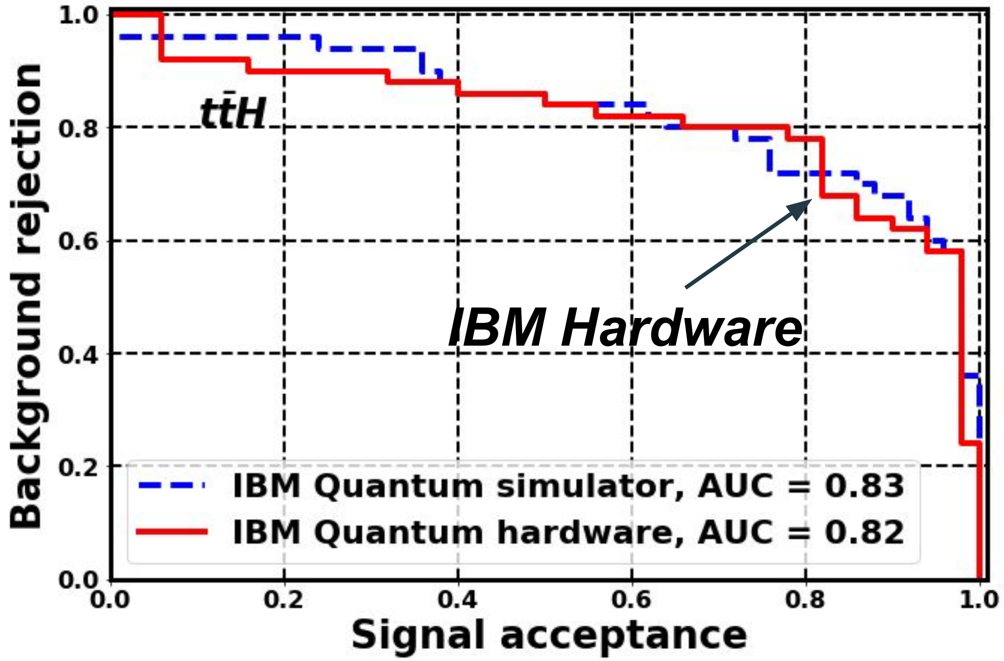
Red: Quantum Hardware

Loss: the mean of the squared differences between the output scores from the quantum algorithm and the ideal scores

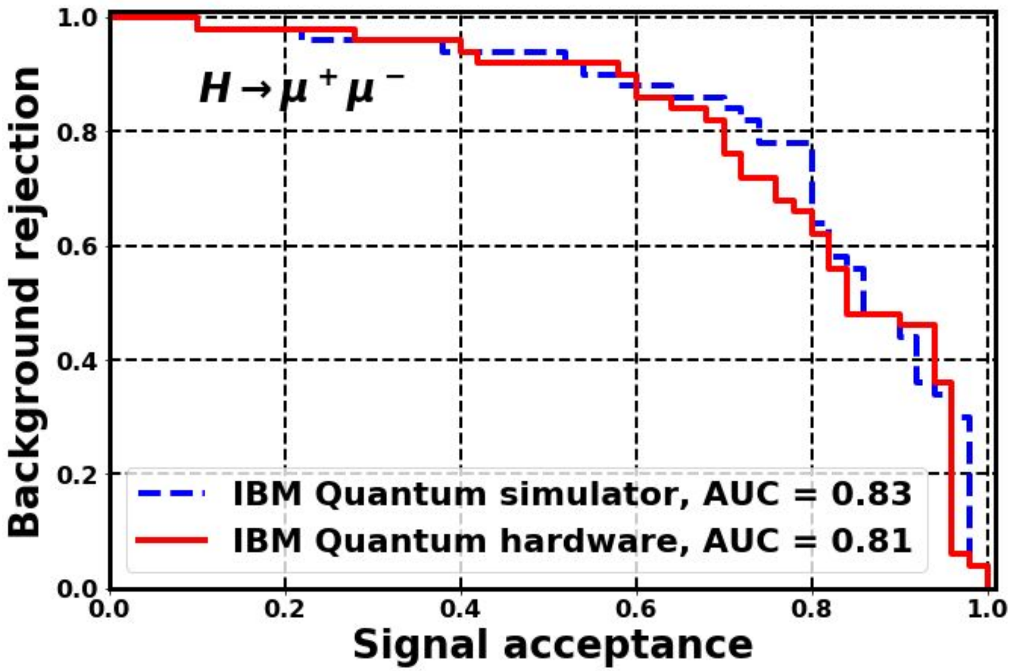
- **The hardware loss (red) is decreasing with the increase of number of iterations*. This indicates that the Quantum Computer has the ability to learn how to differentiate between the signal and the background for a HEP analysis.**

* **“iteration” indicates the number of times the algorithm’s parameters are updated in training**

Method 1: Employing VQC (Variational Quantum Classifier) with IBM hardware for ttH ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis



hardware AUC = 0.82, simulator AUC = 0.83



hardware AUC = 0.81, simulator AUC = 0.83

- **Using ttH analysis dataset (100 events, 10 variables) and $H \rightarrow \mu\mu$ analysis dataset (100 events, 10 variables), with 250 iterations, the result of Variational Quantum Classifier from Quantum Hardware and result from Quantum Simulator are in good agreement.**

* "iteration" indicates the number of times the algorithm's parameters are updated in training

Example 2

Employing Quantum Support Vector Machine (QSVM) Kernel method for ZH ($H \rightarrow \gamma\gamma$) analysis at CEPC

arxiv:2209.12788

Earlier work by Wu et al:

Phys. Rev. Research 3, 033221 (2021)

I am now in an another collaboration for studying Quantum Machine Learning application in High Energy Physics:

Abdualazem Fadol, Zhan Li, Yaquan Fang, Qiyu Sha
Institute of High Energy Physics, Chinese Academy of Sciences

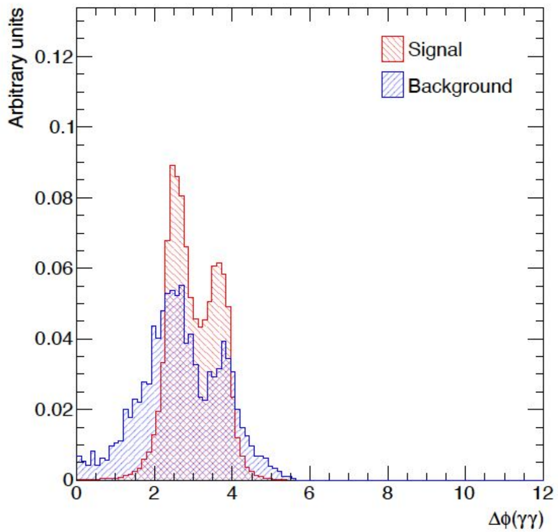
Congqiao Li, Sitian Qian, Yuyang Xiao, Chen Zhou
Peking University

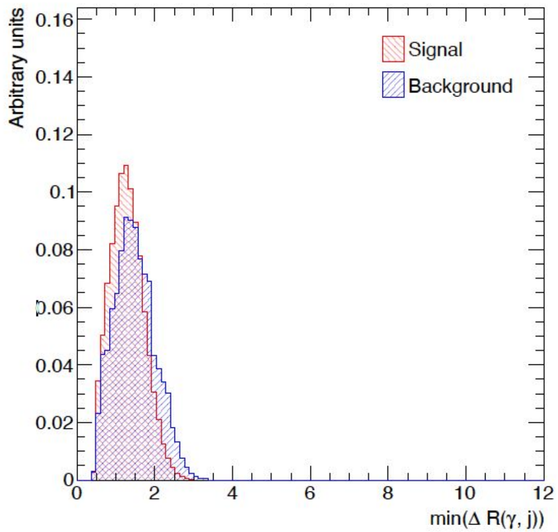
Yu Zhang
Qujing Normal University

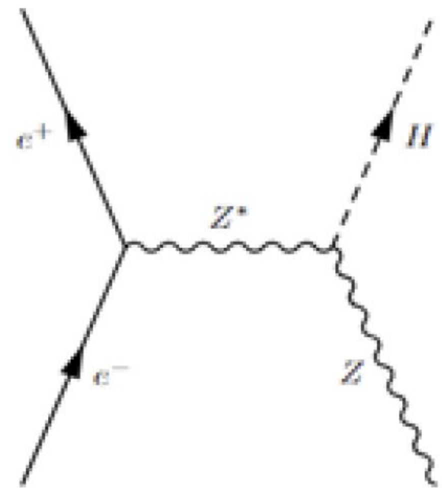
Employing Quantum SVM Kernel methods for future collider (e.g. CEPC) physics analysis

Using QSVM Kernel method, we are performing the CEPC ZH (H→γγ) analysis

- ***ZH is the main Higgs production mode for future electron-positron colliders, providing possibilities for precision measurements of Higgs properties***

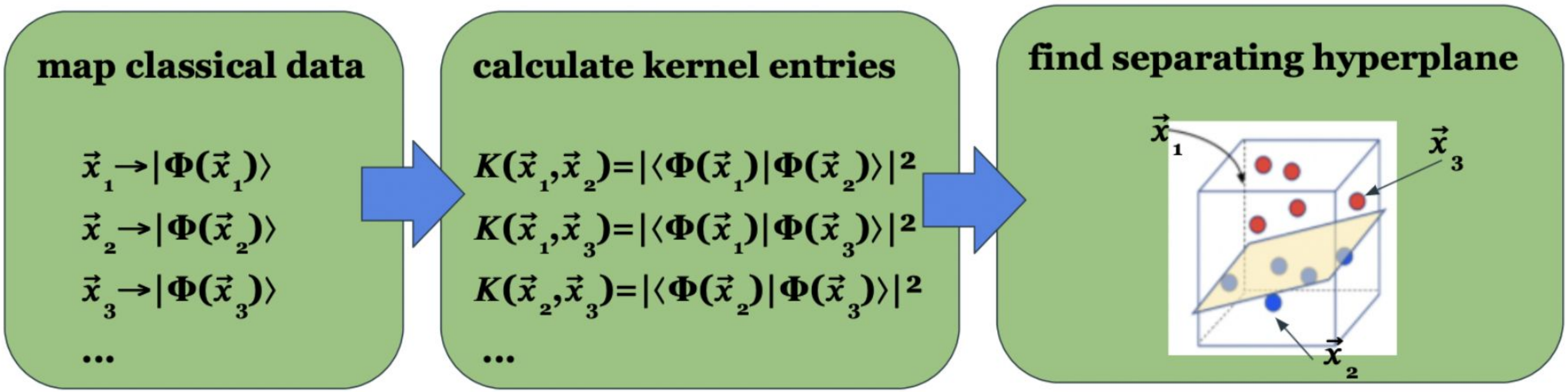






Method 2: Quantum SVM Kernel method

- ***Quantum SVM Kernel method* (introduced by IBM, published in Nature 567 (2019) 209):**
    - ***map classical data $\vec{x}$ to a quantum state $|\Phi(\vec{x})\rangle$ using a Quantum Feature Map function;***
    - ***calculate the similarity between any two data events ("kernel entry") as $K(\vec{x}_1,\vec{x}_2)=|\langle\Phi(\vec{x}_1)|\Phi(\vec{x}_2)\rangle|^2$ using a quantum computer;***
    - ***then using the kernel entries to find an optimal separating hyperplane that separates signal from background.***



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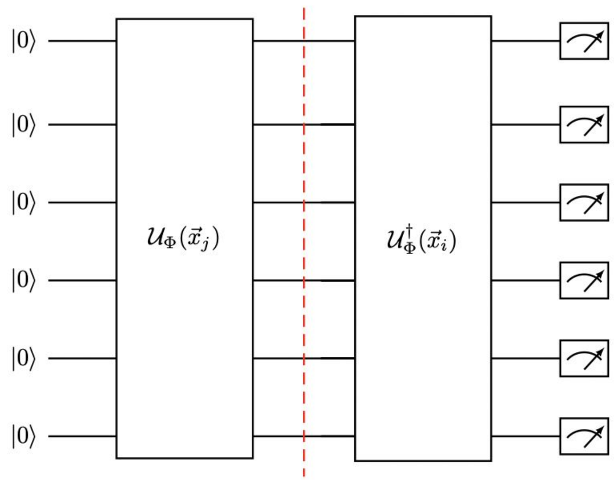
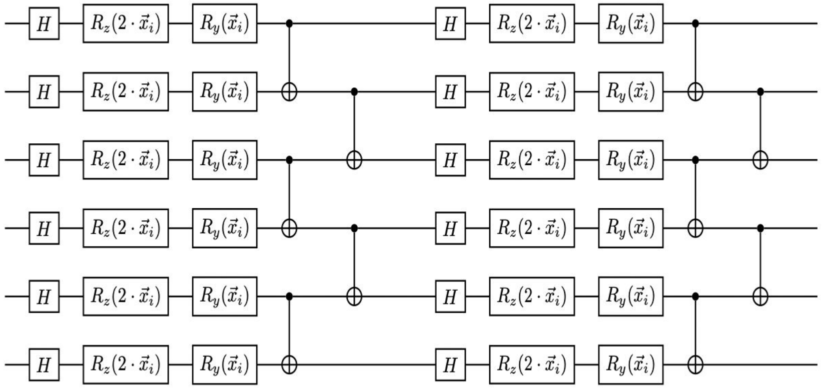


Method 2: Employing Quantum SVM Kernel method with quantum simulators for ZH (H → $\gamma\gamma$) analysis



Rotation	Depth	Events	Best AUC	Variation
$R_z(2\cdot\vec{x}_i)+R_y(\vec{x}_i)$	2	5000	0.935	0.009
$R_z(\vec{x}_i)+R_y(\vec{x}_i)$			0.933	0.015
$R_y(\vec{x}_i)+R_x(\vec{x}_i)$			0.932	0.015
$R_z(\vec{x}_i)+R_z(\vec{x}_i)$			0.932	0.014
$R_y(\vec{x}_i)$			0.928	0.008
$R_z(\vec{x}_i)$			0.928	0.008

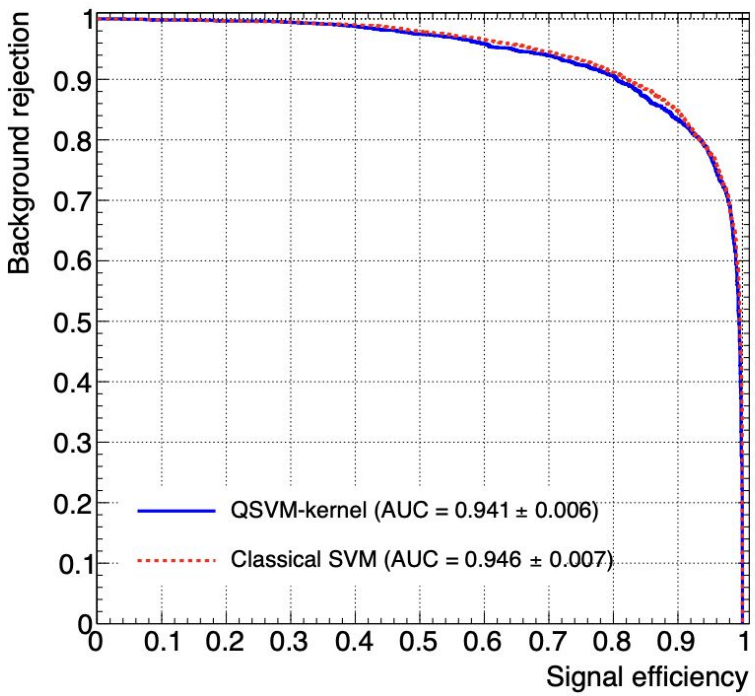
We have performed the ZH analysis using QSVM Kernel method with up to 6 qubits:

- ***A customized FeatureMap is used. The quantum FeatureMap circuit encodes classical data to a quantum state***
- ***Grid-Search with cross-validation* is used to optimize the QSVM Kernel performance***

Method 2: Employing Quantum SVM Kernel method with quantum simulators for ZH ($H \rightarrow \gamma\gamma$) analysis

- ***Our group has implemented the QSVM Kernel algorithm using the Statevector Simulator from the IBM Qiskit framework and the TensorNetwork Simulator from the Origin QPanda framework***
    - ***These simulators represent the ideal quantum hardware that performs infinite measurement shots and experiences no hardware device noise***
    - ***We have overcome the challenges of heavy computing resources in the use of up to 6 qubits and up to 12500 events on the quantum computer simulators***

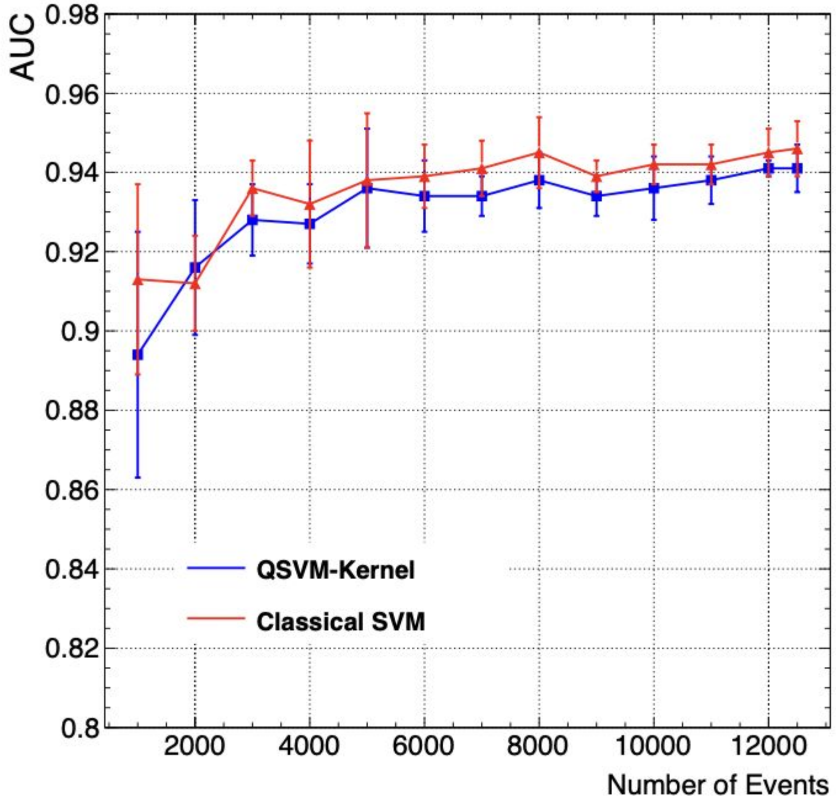
Method 2: Employing Quantum SVM Kernel method with quantum simulators for ZH ($H \to \gamma\gamma$) analysis



- **For 15 qubits, using ttH analysis dataset (12500 events), QSVM Kernel on simulator (blue) achieves similar performances with classical SVM (red) . (Results are averaged over multiple datasets)**

Method 2: Employing Quantum SVM Kernel method with quantum simulators for ZH ($H \rightarrow \gamma\gamma$) analysis

AUC vs number of events



- **QSVM Kernel method and noiseless simulators enable us to work with a larger number of events.**

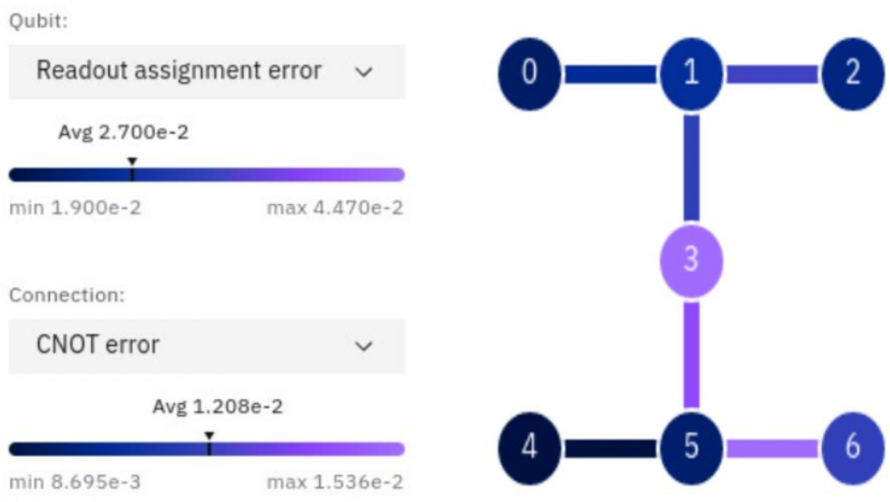
- **For 6 qubits, using ZH analysis dataset (1000-12500 events), QSVM Kernel on simulator (blue) achieves similar performances with classical SVM (red).**

Method 2: Employing QSVM Kernel with IBM and Origin hardware for ZH ($H \to \gamma\gamma$) analysis

- ***We have also been running the QSVM Kernel algorithm on quantum computer hardware provided by both IBM and OriginQ (based on superconducting circuits)***
    - ***to assess the quantum machine learning performances on today's noisy quantum computer hardware***
    - ***due to current limitation of access time on hardware, we only process a dataset of 100 training events and 100 testing events***

Method 2: Employing QSVM Kernel with IBM and Origin hardware for ZH ($H \to \gamma\gamma$) analysis

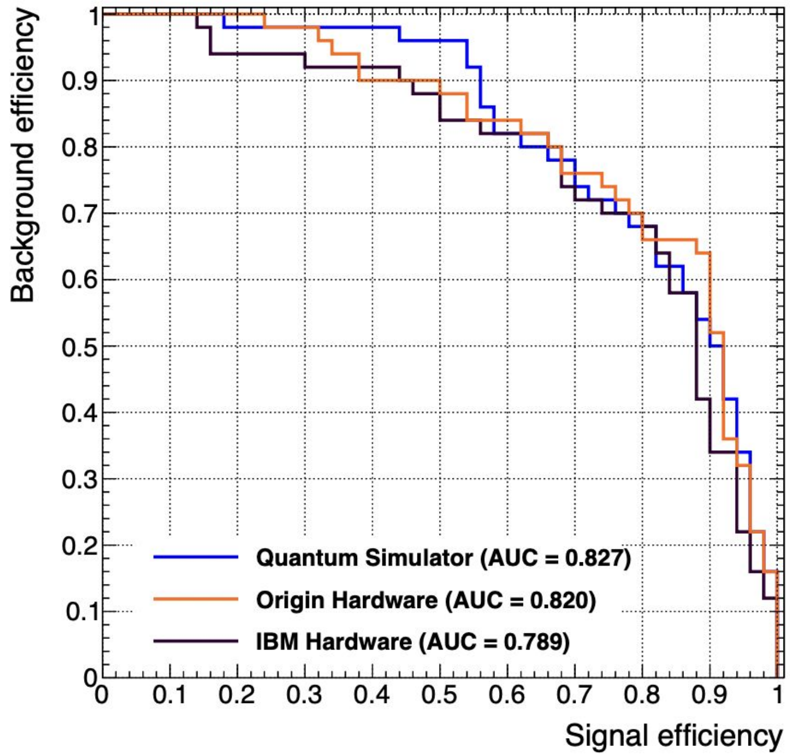
- **Topology structure of the IBM hardware (7 qubits) and OriginQ hardware (6 qubits)**
- **Color indicates some noise level**



(a)

(b)

Method 2: Employing QSVM Kernel with IBM and OriginQ hardware for ZH ($H \rightarrow \gamma\gamma$) analysis



Quantum simulator AUC = 0.827

OriginQ hardware AUC = 0.820

IBM hardware AUC = 0.789

- **Using ZH analysis dataset (100 events, 6 variables), the QSVM Kernel results on the Quantum Hardware (6 qubits) are promising and approaching the QSVM Kernel results on Quantum Simulator (the difference is likely due to statistical fluctuation and effect of hardware noise)**

Challenges ahead

- **Difficulties at present:**
  - **Only ~100 events are used in hardware jobs**
    - **Limited access time and long execulation time**
  - **Only ~10 qubits are used in hardware jobs**
    - **Limited by the hardware noise**
    - **For the same reason, circuit lengths and number of quantum gates are also limited in the present study**
- **To use Quantum Computer Hardware for Machine Learning in High-Luminosity LHC and future collider physics analyses, we need to extend our studies to larger event sample sizes and more qubits**

Opportunities

- Quantum computing industry expect that quantum hardware in the future will reduce noise, increase number of qubits and speed up running time.
- With the large investments in quantum computing and fierce international competitions in technology, this expectation is realistic.
- The HEP community should be well prepared to make use of potential quantum advantage in our data challenge.
- Conversely, applications in HEP could contribute to developments of quantum technologies.

Summary

- Researchers have employed Quantum Machine Learning methods (e.g. Variational Quantum Classifier, Quantum Support Vector Machine Kernel) to LHC and future collider physics analysis
- The results (on both simulators and hardware) demonstrate quantum machine learning on the gate-model quantum computers has the ability to differentiate signal and background in realistic physics datasets

Next steps

- Work with state-of-the-art quantum devices, e.g. Wukong (本源量子) and Kuafu (北京量子院)
- Improve the Quantum SVM algorithms in accuracy and speed, see e.g. Yu Zhang's talk
- Explore other Quantum ML algorithms, see e.g. Abdualazem Fadol's talk
- Develop quantum algorithms and devices inspired by particle physics