

Application of Quantum Machine Learning to HEP Analysis at LHC with four different methods

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**Quantum Computing and Quantum Machine Learning Algorithms for
High Energy Physics, BNL**

Our program with Quantum Machine Learning

Our Goal:

To perform LHC 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.

Our present program is to employ the following four quantum machine learning methods:

Method 1. Variational Quantum Classifier Method

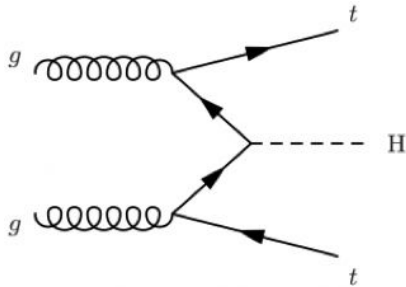
Method 2. Quantum Support Vector Machine (QSVM) Kernel Method

Method 3. Quantum Neural Network Method

Method 4. Quantum DeepSets Method

to LHC High Energy Physics analysis, for example ttH ($H \rightarrow \gamma\gamma$) and $H \rightarrow \mu\mu$ (two LHC flagship analyses).

Employ Quantum Machine Learning to LHC High Energy Physics analyses, for example ttH ($H \rightarrow \gamma\gamma$) and $H \rightarrow \mu\mu$

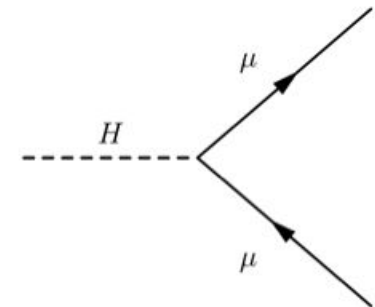


ttH ($H \rightarrow \gamma\gamma$) analysis at the LHC

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

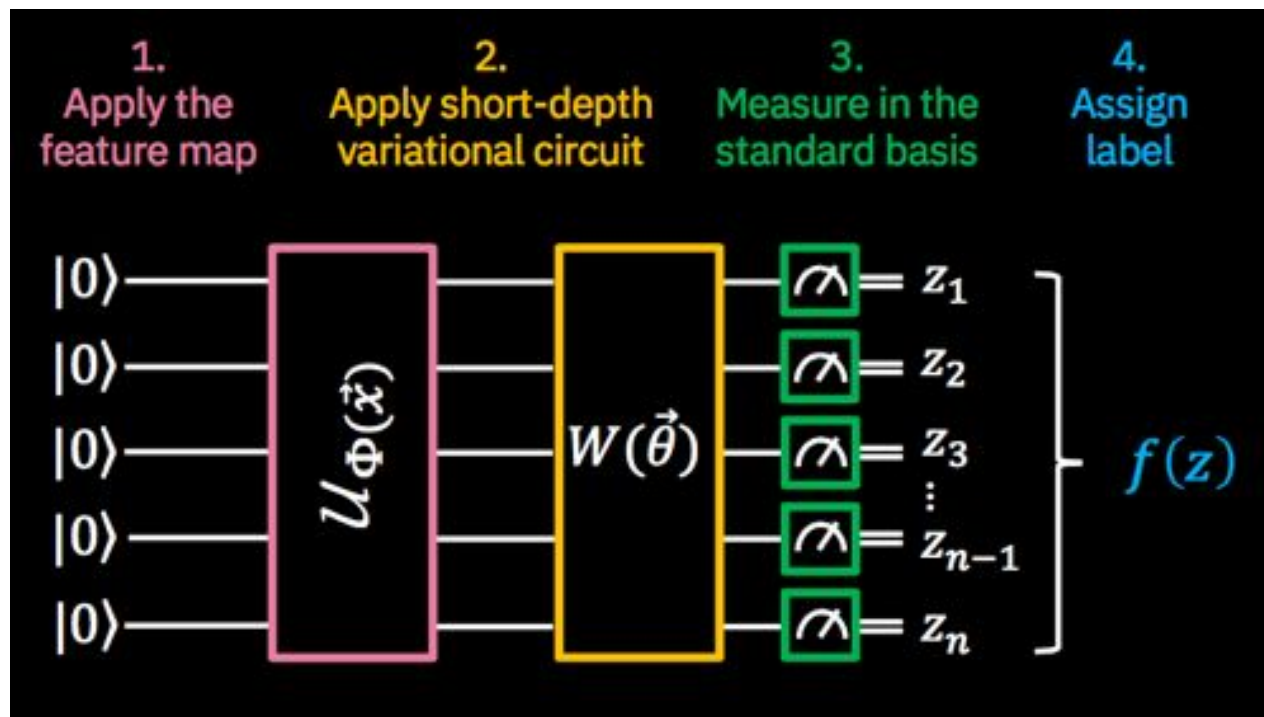
$H \rightarrow \mu\mu$ analysis at the LHC

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. $H \rightarrow \mu\mu$ is the most promising process to observe such a coupling by ATLAS and CMS at the LHC

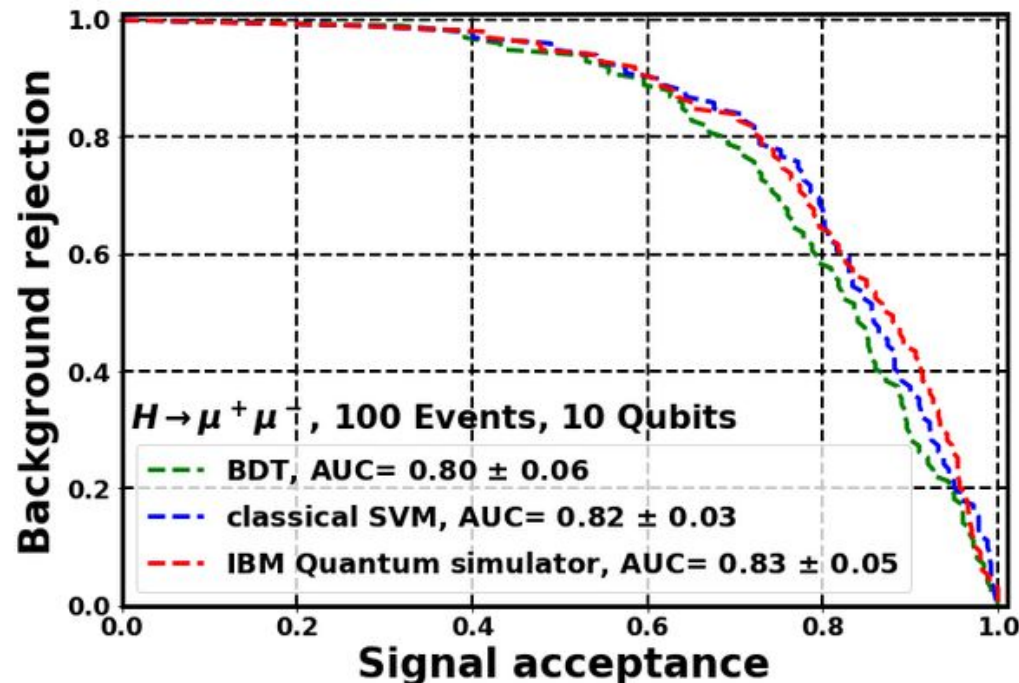
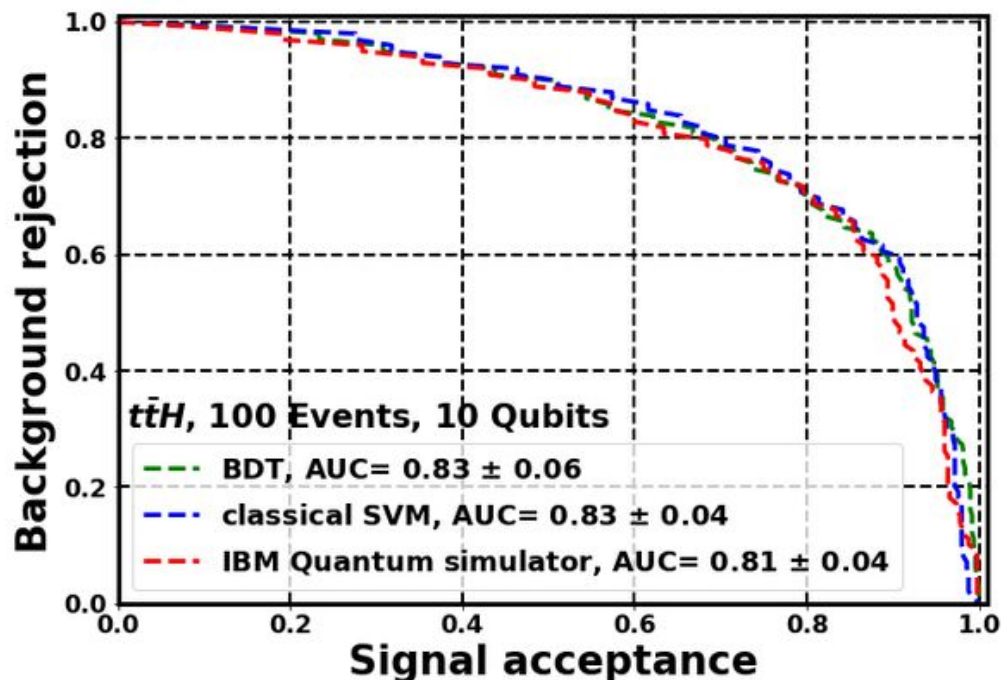


Method 1: Employing Variational Quantum Classifier to ttH ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis

- *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:*



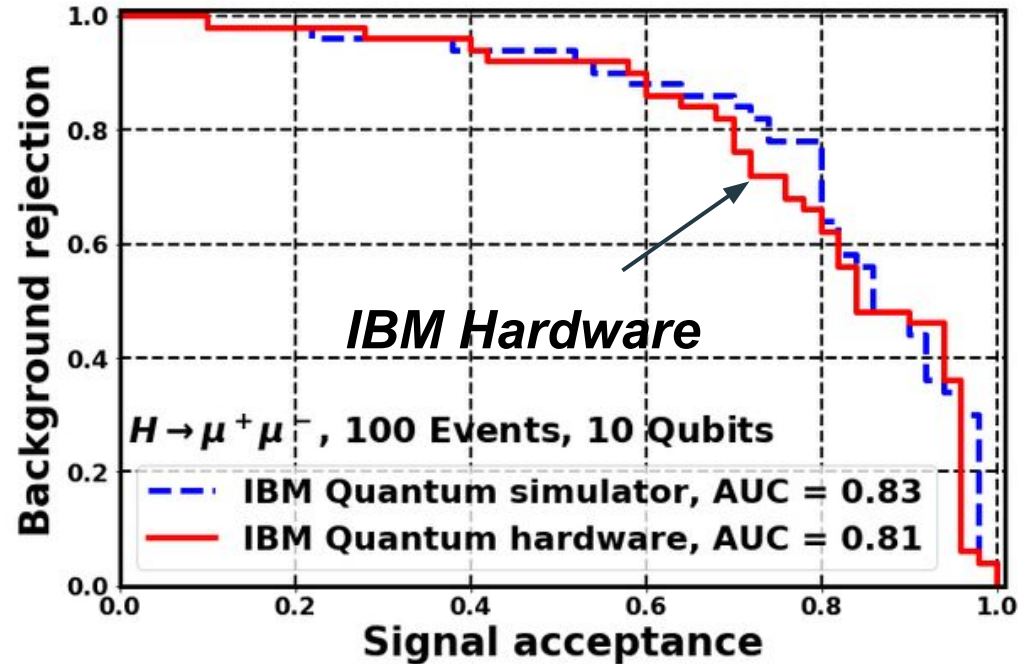
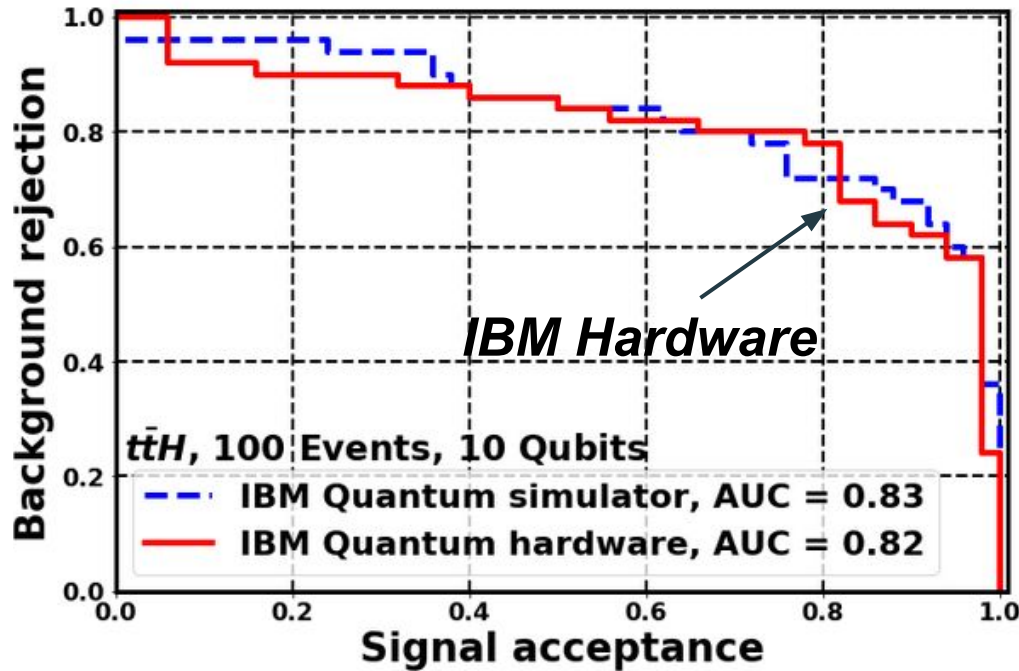
Method 1: Employing VQC (Variational Quantum Classifier) with IBM Q simulator for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis



For 10 qubits, using $t\bar{t}H$ analysis dataset (100 events) and $H \rightarrow \mu\mu$ analysis dataset (100 events), **Variational Quantum Classifier on IBM simulator (red)** performs similarly with **classical BDT (green)** and **classical SVM (blue)**.

	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 $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis



hardware AUC = 0.82, simulator AUC = 0.83

hardware AUC = 0.81, simulator AUC = 0.83

- For 10 qubits, using $t\bar{t}H$ analysis dataset (100 events) and $H \rightarrow \mu\mu$ analysis dataset (100 events), the result of Variational Quantum Classifier from **IBM Quantum Hardware** and result from **Quantum Simulator** are in good agreement.
- **The hardware running time for 100 events is 200 hours**

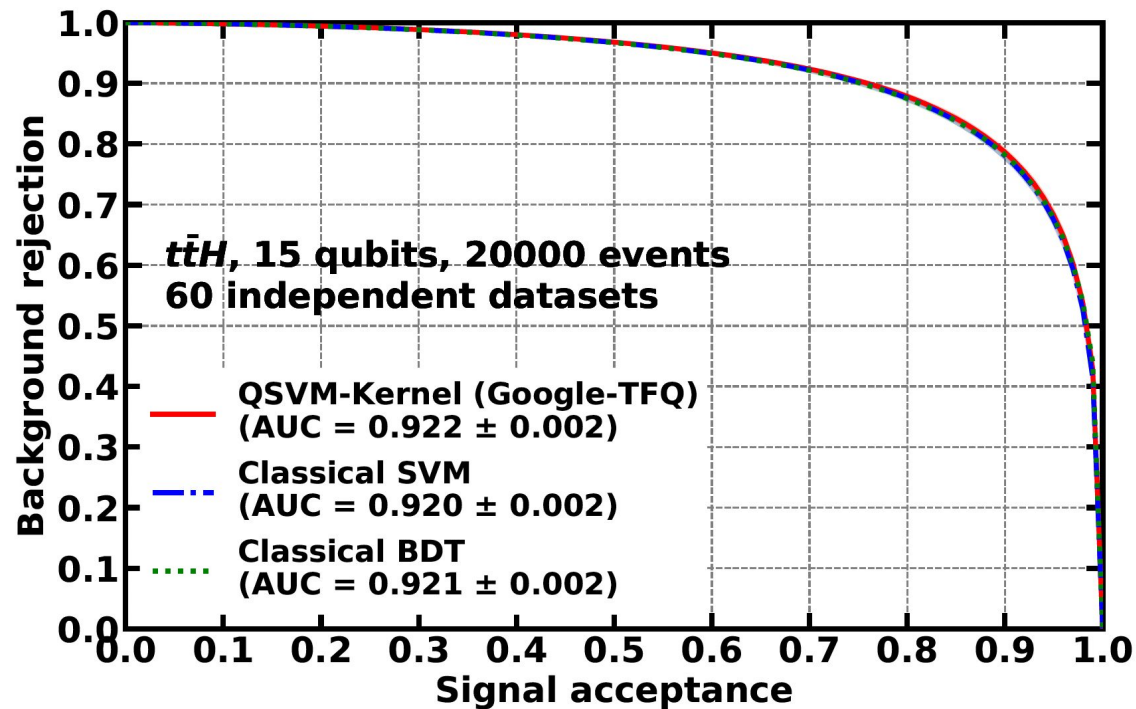
***Method 2: Employing Quantum Support Vector
Machine Kernel method to ttH ($H \rightarrow \gamma\gamma$) analysis***

Method 2: Quantum Support Vector Machine (QSVM) Kernel method

QSVM Kernel method (introduced by IBM, published in *Nature* 567 (2019) 209):

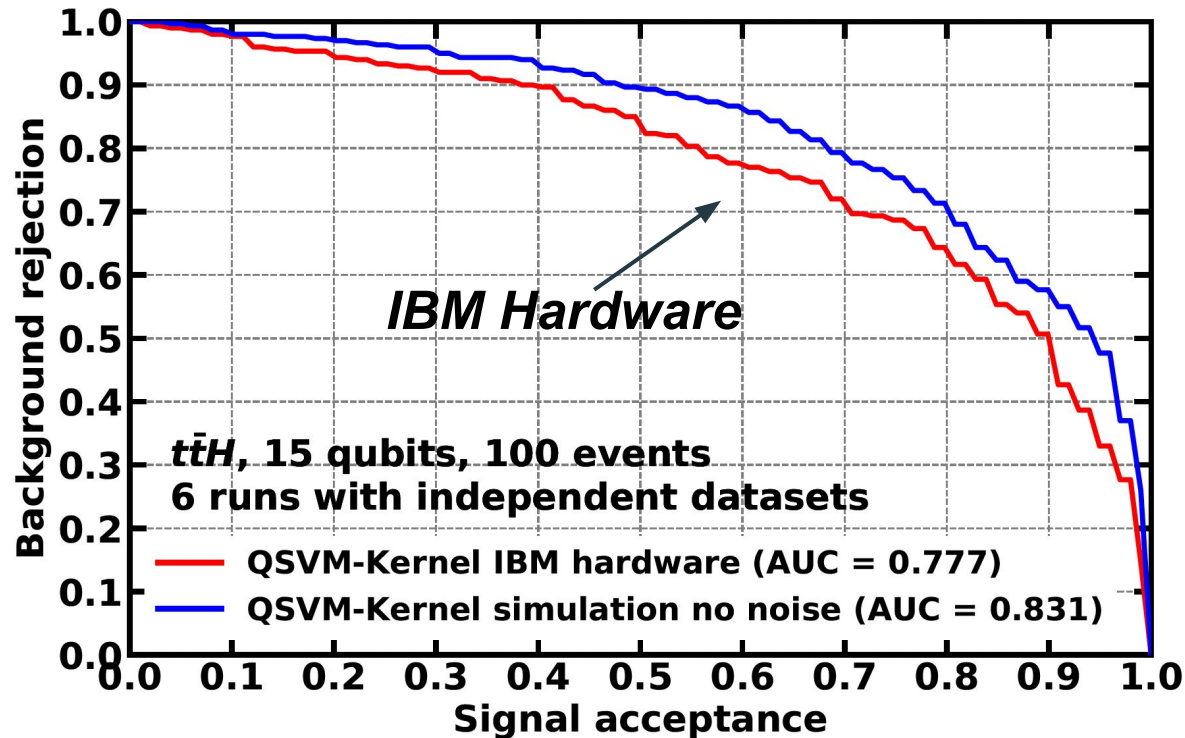
- *map classical data \vec{x} to a quantum state $|\Phi(\vec{x})\rangle$ using a Quantum Feature Map function;*
- *calculate the kernel matrix between any two data events as $K(\vec{x}_1, \vec{x}_2) = |\langle \Phi(\vec{x}_1) | \Phi(\vec{x}_2) \rangle|^2$ using a quantum computer;*
- *then train the Quantum SVM the same way as a classical SVM.*

Method 2: Employing QSVM Kernel with quantum simulators for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



- For 15 qubits, using $t\bar{t}H$ analysis dataset (20000 events), **QSVM Kernel on simulator (red)** achieves similar performances with **classical SVM (blue)** and **classical BDT (green)**.

Method 2: Employing QSVM Kernel with *ibmq_paris*, a 27-qubit machine for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



hardware AUC = 0.777

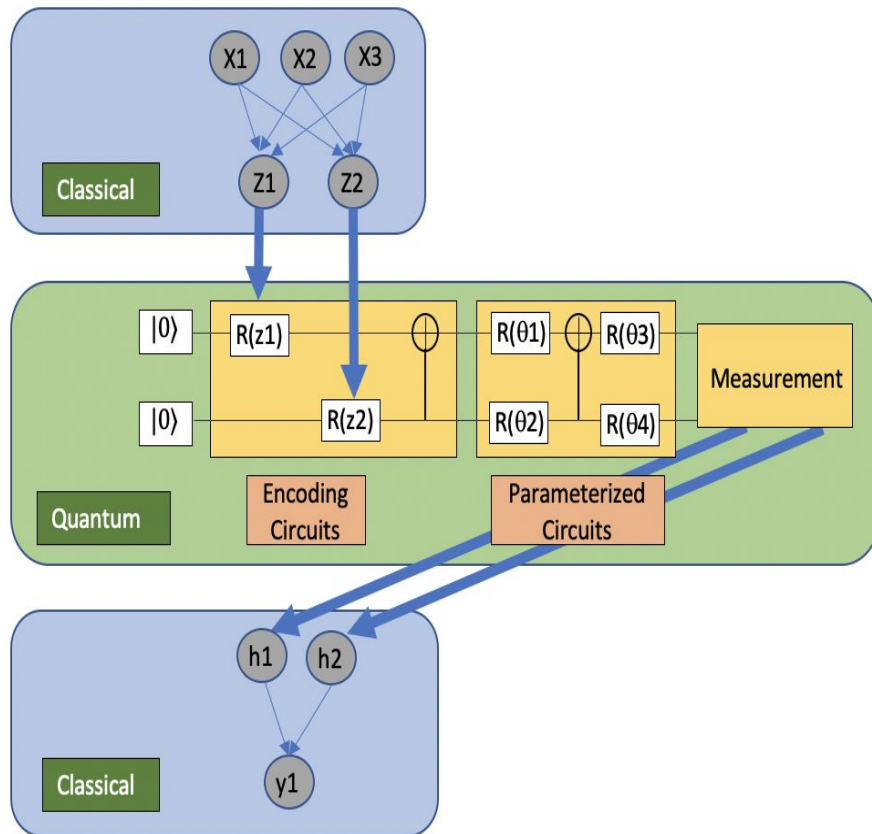
simulator AUC = 0.831

- Using $t\bar{t}H$ analysis dataset (100 events), the **QSVM Kernel results on the IBM Quantum Hardware (15 qubits)** are promising and approaching the **QSVM Kernel results on Quantum Simulator** (the difference is likely due to effect of hardware noise)
- *The average hardware running time for 100 events is approximately 11 hours per run compared with 200 hours for 100 events in method 1.*

***Method 3: Employing Quantum Neural Network
for ttH ($H \rightarrow \gamma\gamma$) analysis***

Method 3: Hybrid Quantum Neural Network (QNN)

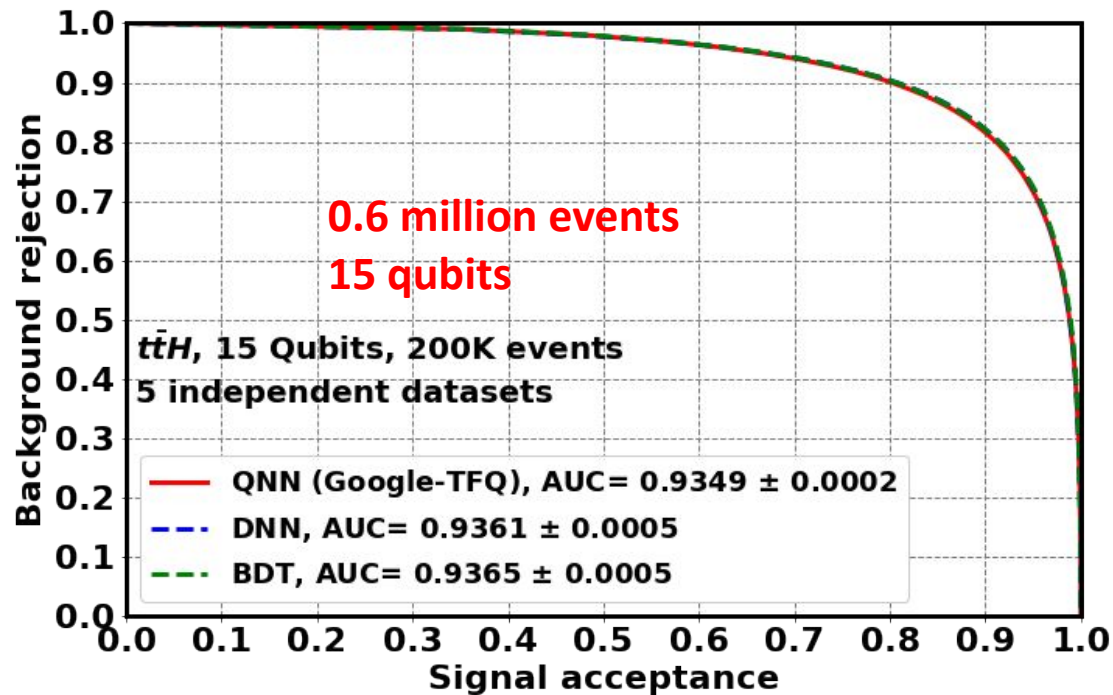
We have been exploring a hybrid QNN of three layers:



- **Classical layer 1:** transform input data so that its number of outputs matches number of qubits (PCA is no longer necessary)
- **Quantum layer (*the core part*):** encode classical data into a quantum state, apply variational circuit containing trainable parameters, and measure the quantum state
- **Classical layer 2:** convert the measurement of qubits to classification labels

Three layers are trained together to maximize the overall performance

Method 3: Employing QNN with Google simulator for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



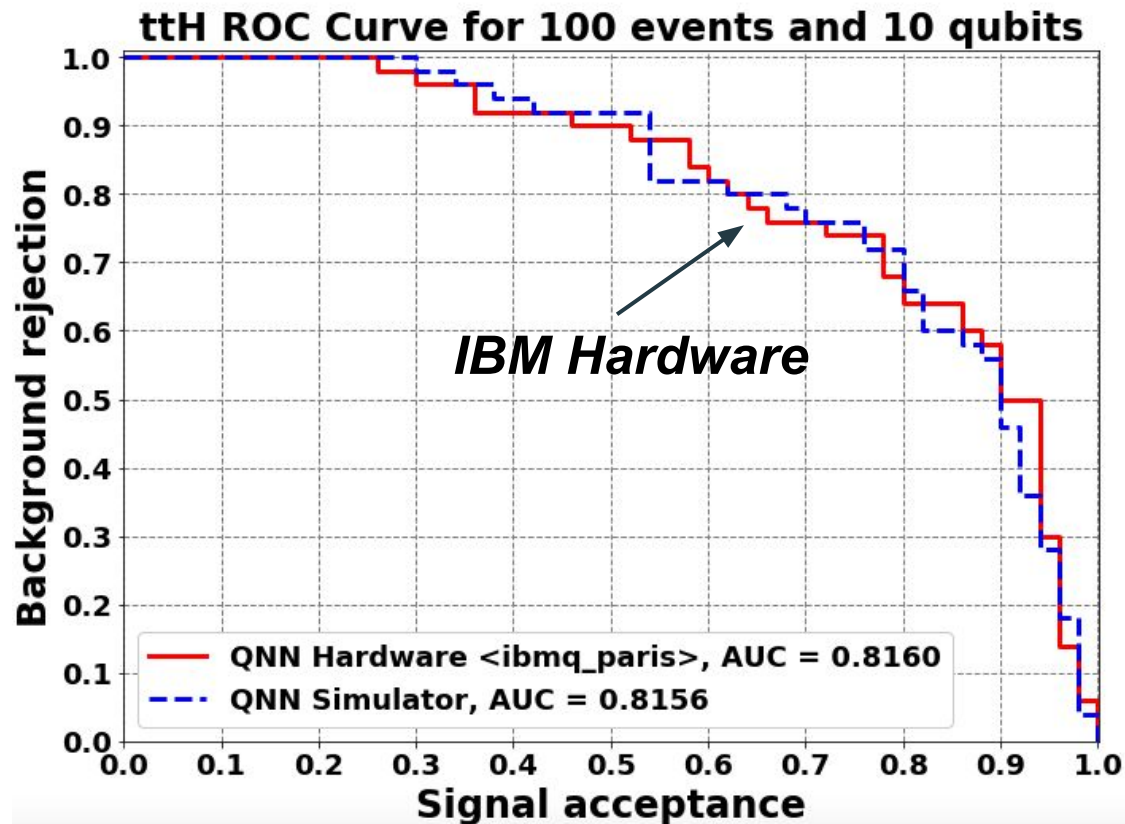
QNN AUC: 0.9349

DNN AUC: 0.9361

BDT AUC: 0.9365

- Using the $t\bar{t}H$ analysis dataset with 0.6 million Delphes events (in total) and 15 qubits, **QNN on Google simulator (red)** now performs similarly with **classical Deep Neural Network (DNN) (blue)** and **classical BDT (green)**.
- The optimization of this QNN is still under development (e.g. more qubits), and we hope to achieve quantum advantage with large datasets.

Method 3: Employing QNN with IBM Q hardware (10 qubits) for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



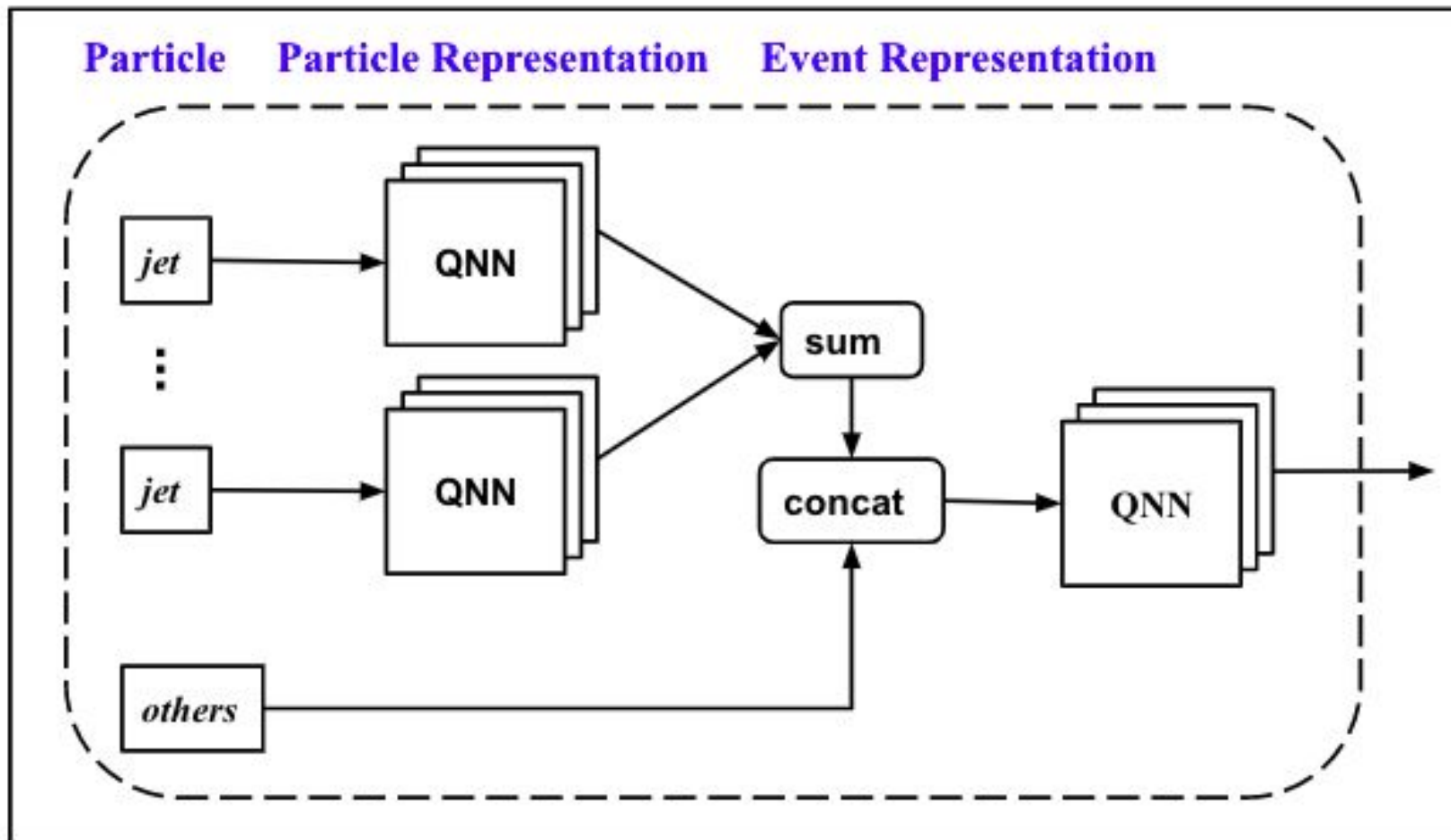
- 100 events, 10 qubits, 1 run

	AUC (100 events)
Hardware	0.816
Simulator	0.816

- The performance with quantum hardware is close to the performance with no-noise simulation.
- Hardware running time for 100 events: 384 hours

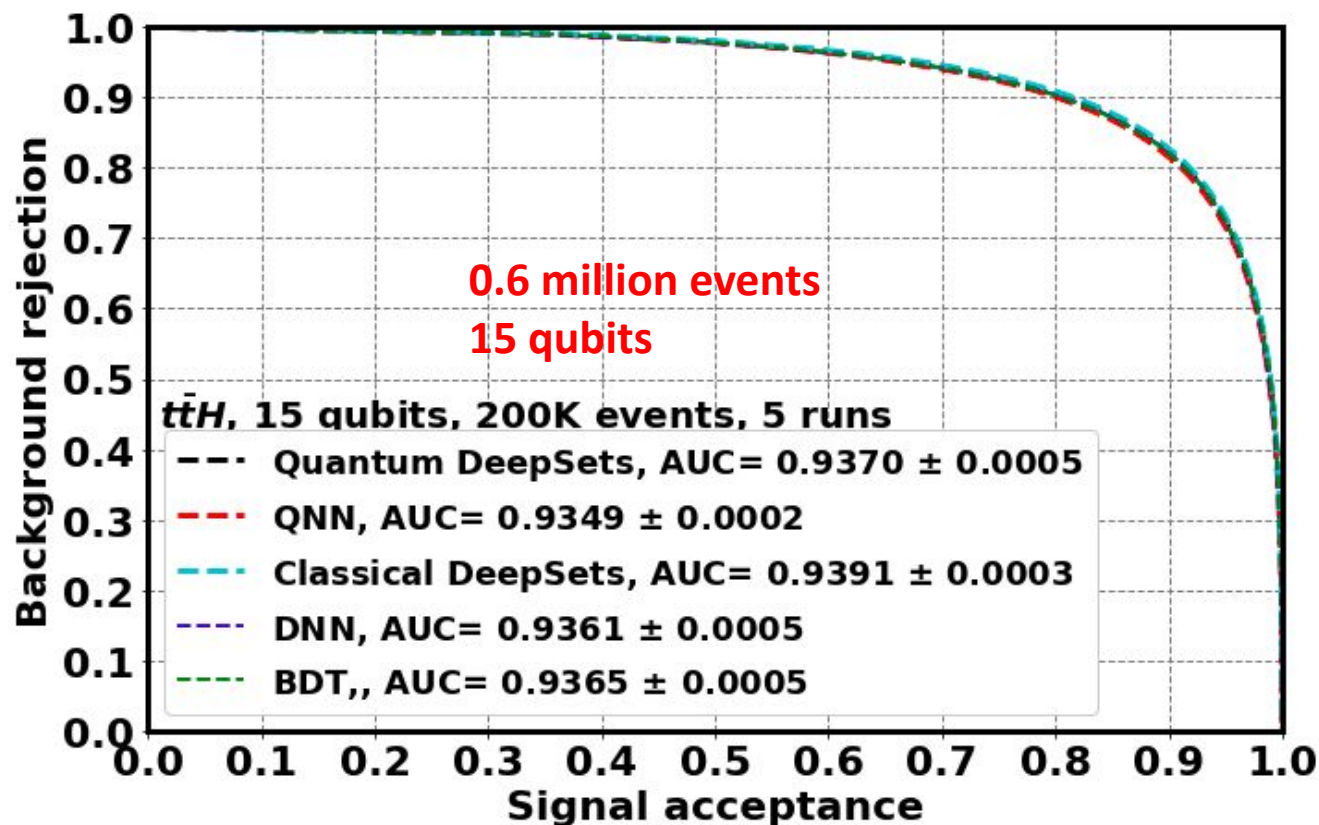
***Method 4: Employing Quantum Deepsets for $t\bar{t}H$
($H \rightarrow \gamma\gamma$) analysis***

Method 4: Quantum Deepsets



- *Each jet is mapped to a particle representation by a quantum neural network;*
- *The summed particle representations concatenated with other particle variables arrive at an event representation;*
- *The classification is then performed on the event representation by a quantum neural network.*

Method 4: Employing Quantum DeepSets with Google simulator for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



Quantum DeepSets AUC: 0.9370

QNN AUC: 0.9349

Classical DeepSets AUC: 0.9391

DNN AUC: 0.9361

BDT AUC: 0.9365

- Using the $t\bar{t}H$ analysis dataset with 0.6 million Delphes events (in total) and 15 qubits, **QNN (red)** and Quantum DeepSets (black) on Google simulator performs similarly with **classical DeepSets (light blue)**, **DNN (blue)** and **BDT (green)**.

Summary (part 1)

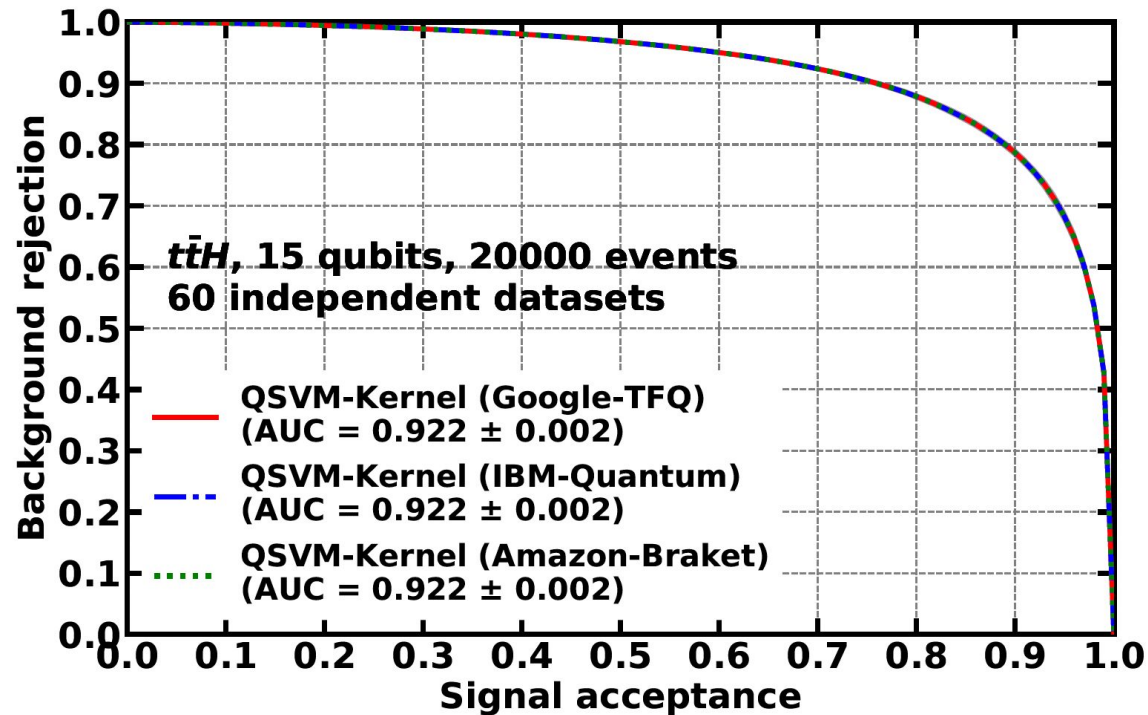
- **We have employed four Quantum Machine Learning methods to two LHC HEP flagship analyses (ttH ($H \rightarrow \gamma\gamma$) and $H \rightarrow \mu\mu$) with Delphes simulation events, and their performs on quantum simulators are similar as the classical ML methods.**
 - **Method 1: VQC-Variational Quantum Classifier**
(J. Phys. G: Nucl. Part. Phys 48, 125003, 2021)
 - **Method 2: QSVM Kernel method** (*Phys. Rev. Research 3, 033221, 2021*)
 - **Method 3: Quantum Neural Network** (*in progress*)
 - **Method 4: Quantum Deepsets** (*in progress*)
- **For quantum hardware results, our present studies were limited to 100 events and 10-15 qubits because of the limited access time as well as the limitations on circuit length and number of CNOT gates.**

Summary (part 2)

- ***Our 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 step:***
 - We are now working on the NERSC-Perlmutter supercomputer in order to run large number of qubits simulation (20-30 qubits) with GPUs.***

BACKUP SLIDES

Method 2: Employing Quantum Kernel Estimator with quantum simulators for $t\bar{t}H$ ($H \rightarrow \gamma\gamma$) analysis



- For 15 qubits, using $t\bar{t}H$ analysis dataset (20000 events), **Google qsim simulator (red)**, **IBM statevector simulator (blue)**, and **Amazon local simulator (green)** provide identical performances for QSV Kernel method