Application of Quantum Machine Learning to HEP Analysis at LHC using Quantum Computer Simulators and Quantum Computer Hardware – Challenges and Opportunities

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Machine Learning for High Energy Physics

- Classical Machine learning algorithms commonly used in High Energy Physics data analysis
  - Boosted Decision Tree (BDT): an algorithm that incrementally builds an ensemble of decision trees and combines all the decision trees to form a strong classifier.
  - Support Vector Machine (SVM): it maps the input vectors X into a high-dimensional feature space Z through some nonlinear mapping, chosen a priori. In this space, an optimal separating hyperplane is constructed to separate signal from background.
  - Neural Network (NN): a computing system made up of a number of simple, highly interconnected processing elements, which process information by their response to external inputs.

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, as a proof of principle

Our present program is to employ the following 3 quantum machine learning methods

Method 1. Variational Quantum Classifier Method

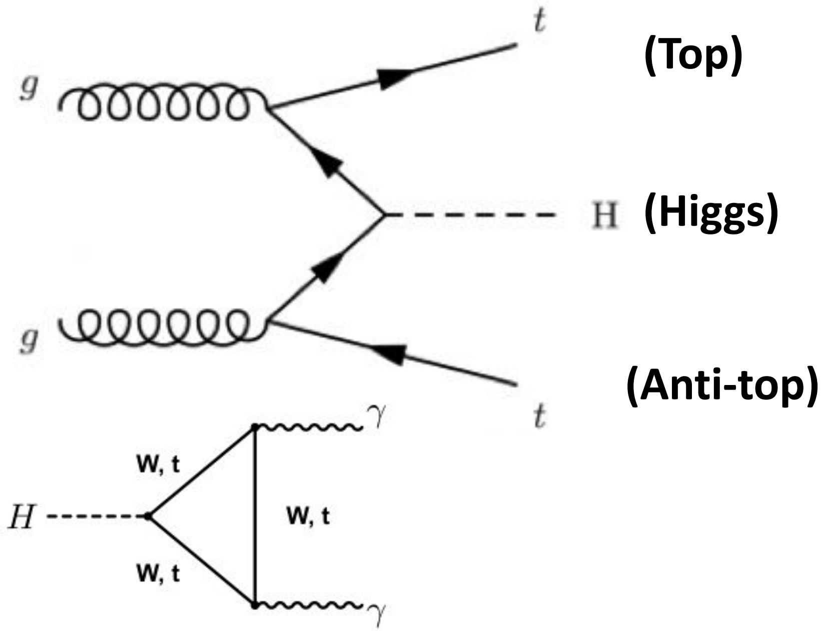
Method 2. Quantum Support Vector Machine Kernel Method

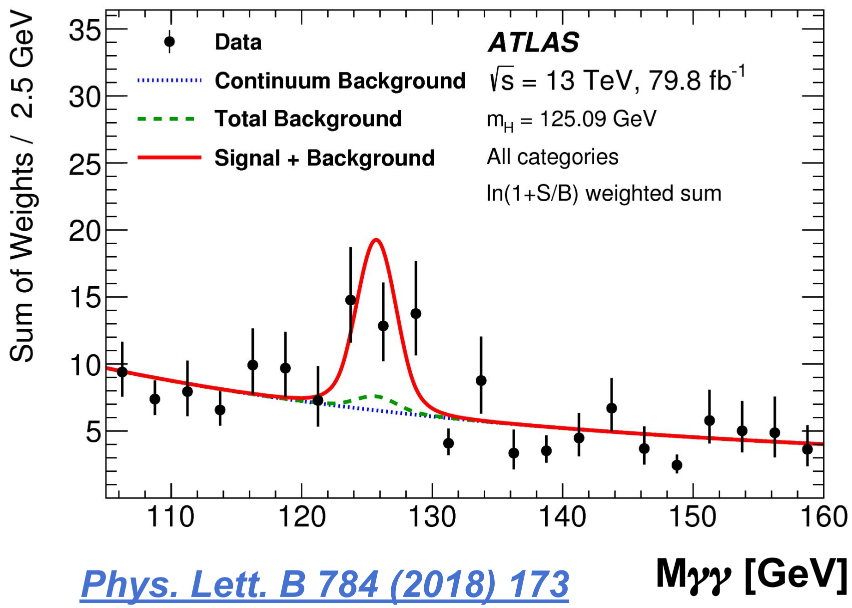
Method 3. Quantum Neural Network Method

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

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





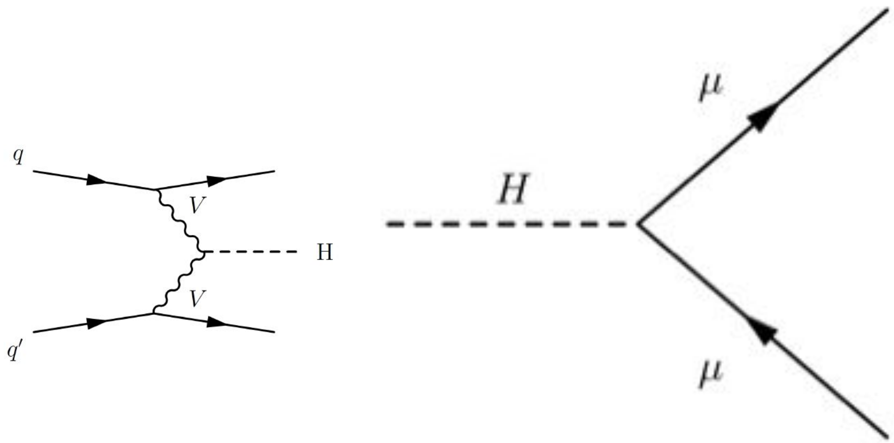
Phys. Lett. B 784 (2018) 173

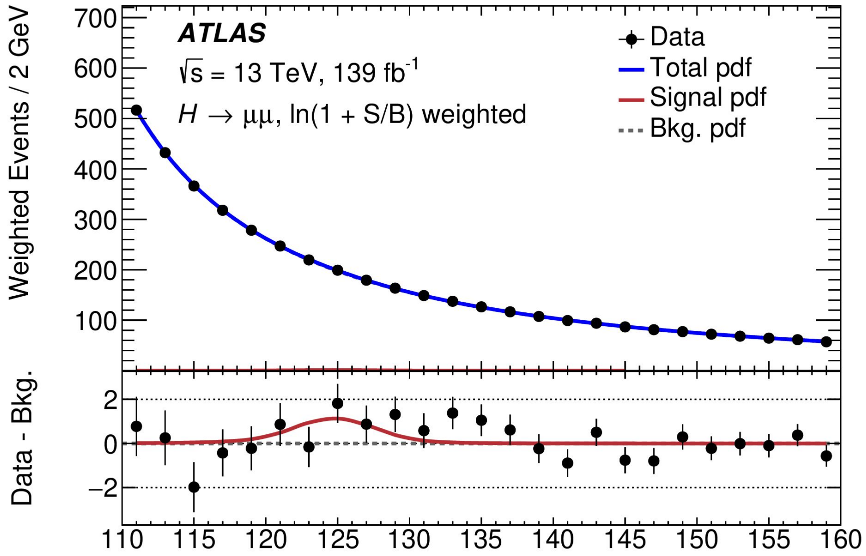
- **Using Boosted Decision Tree (BDT, a classical machine learning technique) with XGBoost package, the ATLAS Collaboration observes the ttH (H→γγ) process**
- **Our study performs the event classification of the ttH (H→γγ) analysis (hadronic channel) with delphes simulation samples and quantum machine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

ATLAS: 2.0σ, Phys. Lett. B 812, 135980 (2021)
CMS: 3.0σ, JHEP 01 148 (2021)





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

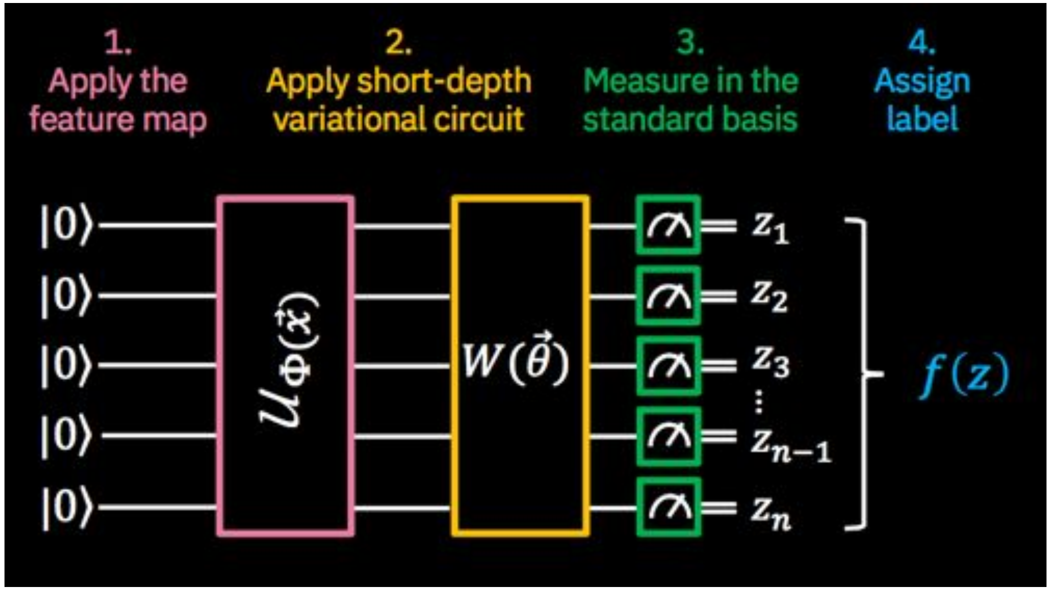
Employing Variational Quantum Classifier for ttH ($H \rightarrow \gamma\gamma$) and $H \rightarrow \mu\mu$ analyses

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)

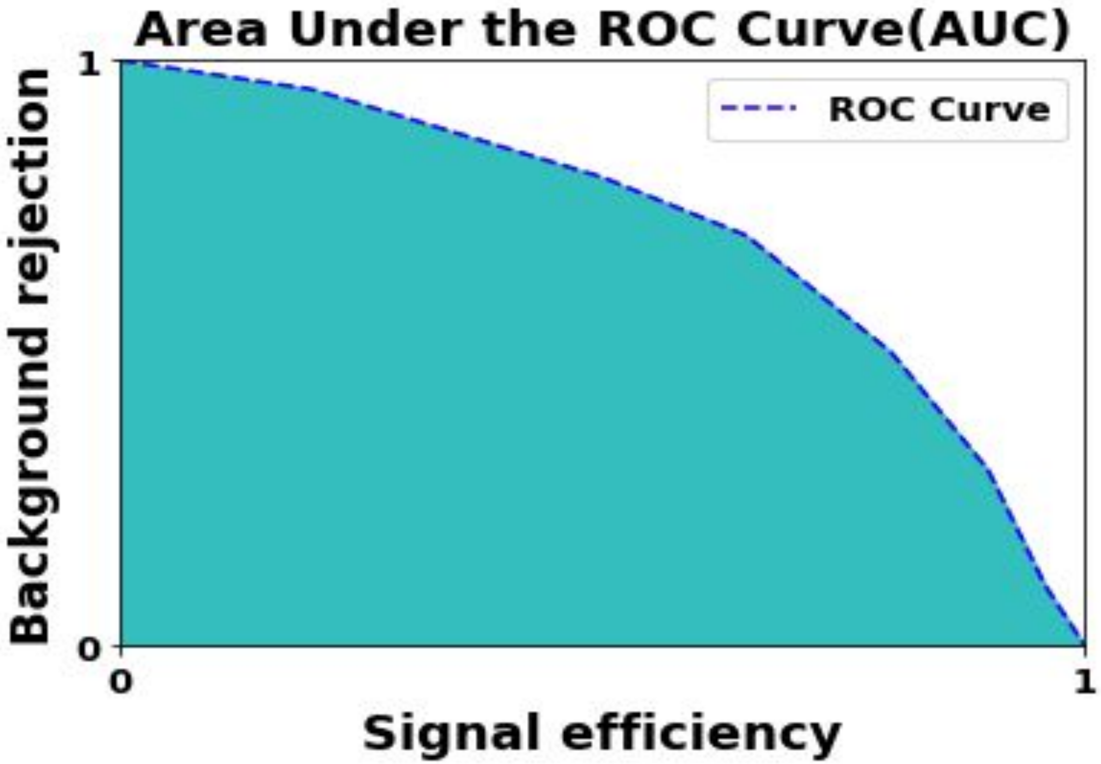
- 1. Apply feature map circuit $U_{\Phi(\vec{x})}$ to encode input data $\vec{x}$ into quantum state $|\Phi(\vec{x})\rangle$
- 2. Apply short-depth quantum variational circuit W(θ) which is parameterized by gate angles θ
- 3. Measure the qubit state in the standard basis (standard basis: $|0\rangle$, $|1\rangle$ 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



- We have two independent sets of events: one for training and one for testing
- 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

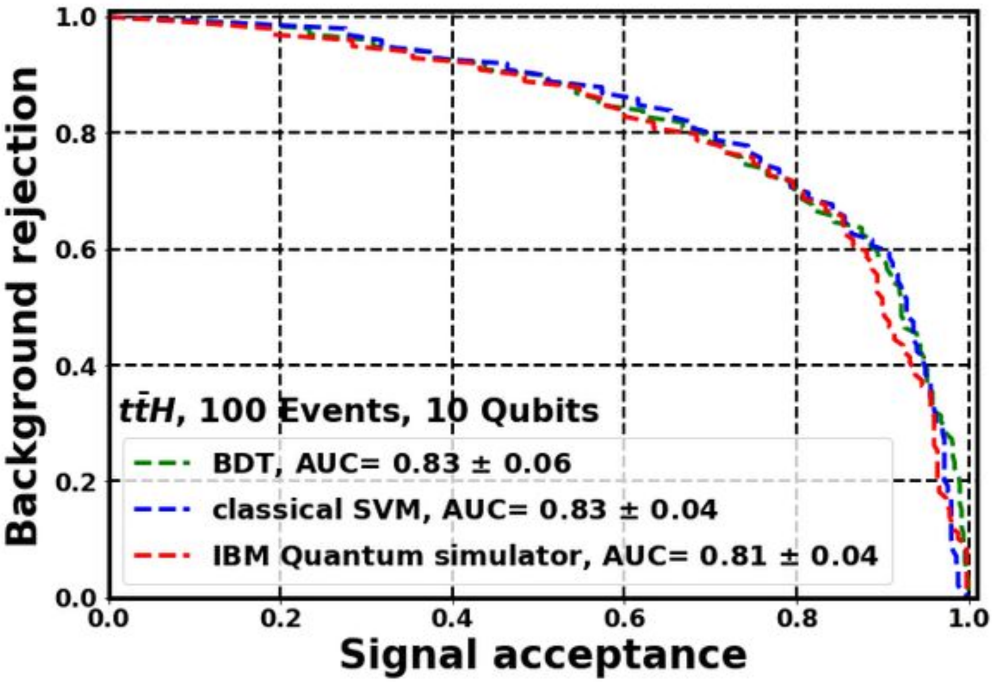
Method 1: Employing VQC (Variational Quantum Classifier) with IBM Q simulator for ttH ($H \rightarrow \gamma\gamma$) analysis and $H \rightarrow \mu\mu$ analysis

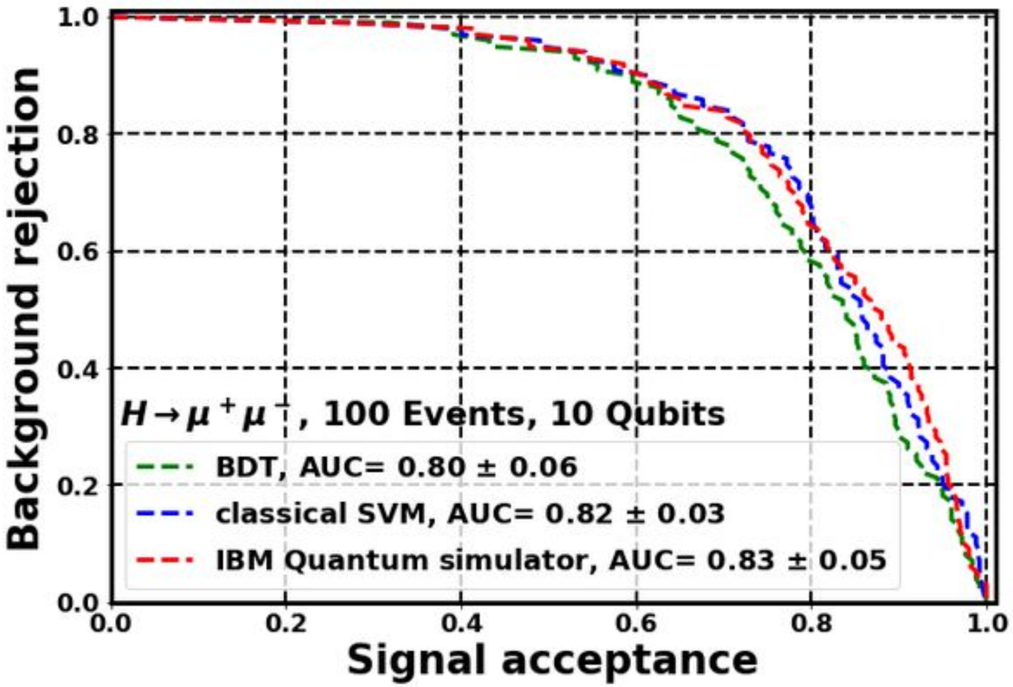
- **Definitions**
  - **ROC (Receiver Operating Characteristic) Curve**: a graph showing background rejection vs signal efficiency.
  - **AUC**: Area Under the ROC Curve, for quantifying discrimitation power of machine learning algorithms



ROC curves and AUC are standard metrics for machine learning applications

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

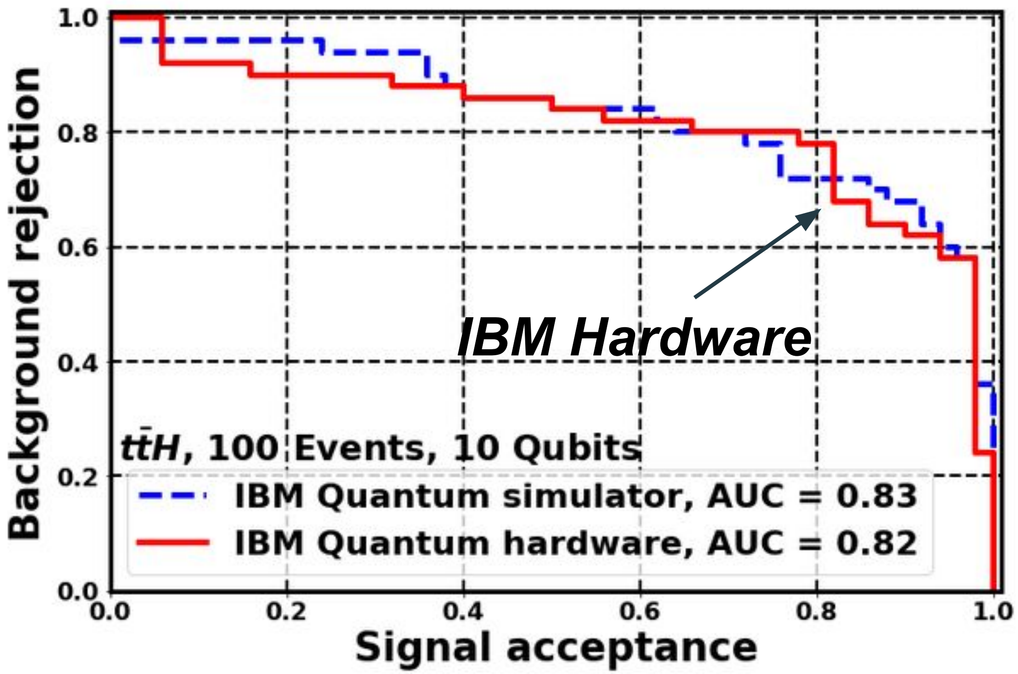




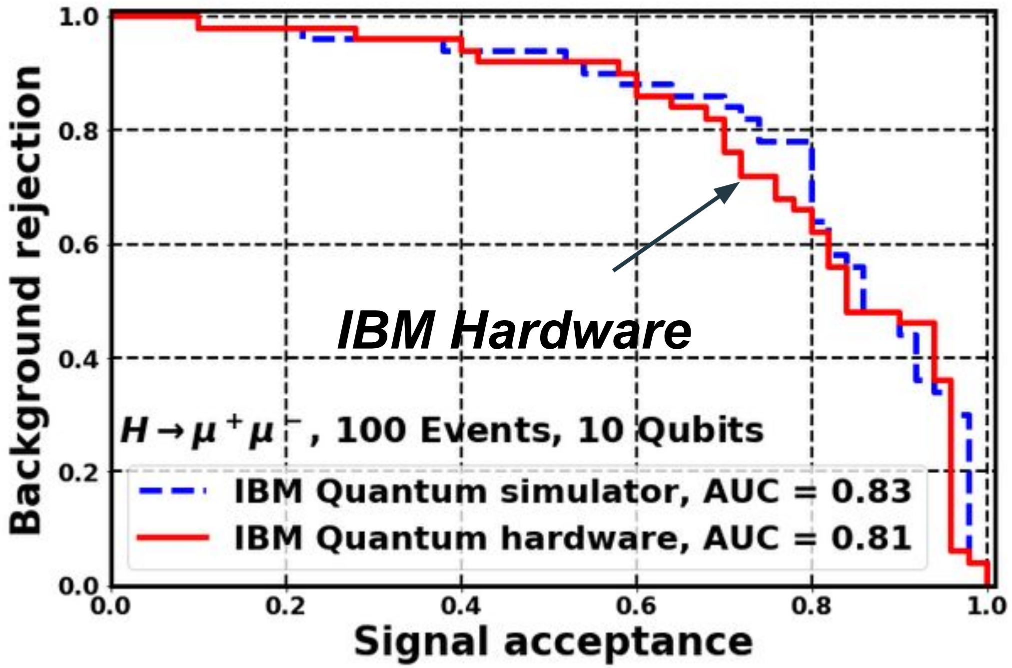
For 10 qubits, using ttH analysis dataset (100 events) and $H \rightarrow \mu\mu$ analysis dataset (100 events), Variational Quantum Classifier on IBM simulator (red) performs similarly with classical BDT (green) and classical SVM (blue).

	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 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

- For 10 qubits, using ttH 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 (QSVM) Kernel method for ttH (H $\rightarrow \gamma\gamma$) analysis

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.***

map classical data

$\vec{x}_1 \rightarrow |\Phi(\vec{x}_1)\rangle$

$\vec{x}_2 \rightarrow |\Phi(\vec{x}_2)\rangle$

$\vec{x}_3 \rightarrow |\Phi(\vec{x}_3)\rangle$

…

calculate kernel entries

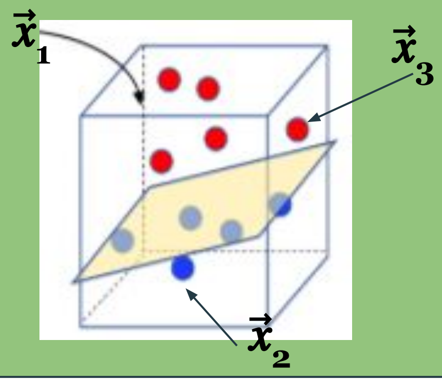
$K(\vec{x}_1,\vec{x}_2)=|\langle\Phi(\vec{x}_1)|\Phi(\vec{x}_2)\rangle|^2$

$K(\vec{x}_1,\vec{x}_3)=|\langle\Phi(\vec{x}_1)|\Phi(\vec{x}_3)\rangle|^2$

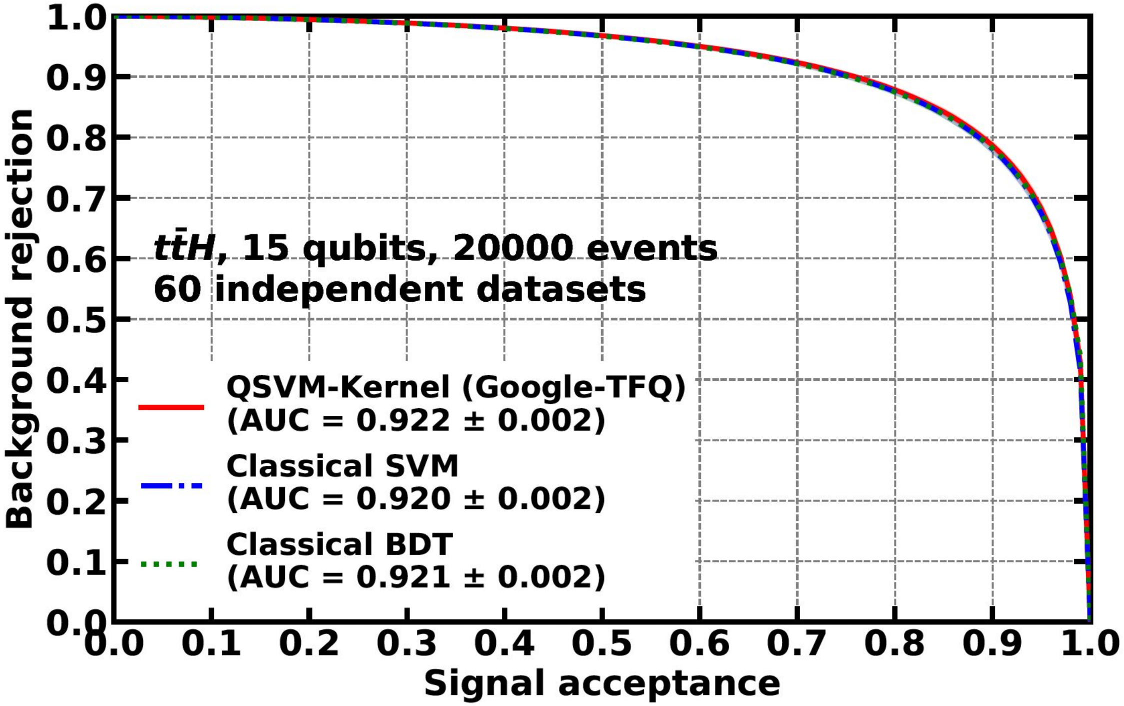
$K(\vec{x}_2,\vec{x}_3)=|\langle\Phi(\vec{x}_2)|\Phi(\vec{x}_3)\rangle|^2$

…

find separating hyperplane

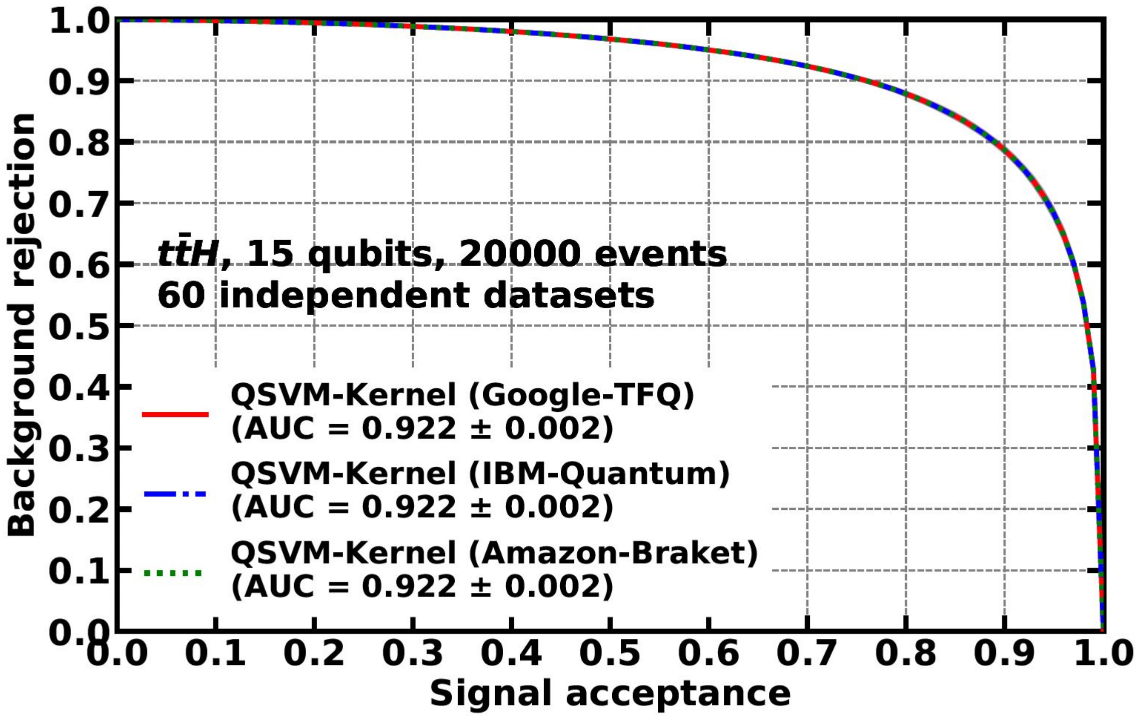


Method 2: Employing Quantum SVM Kernel method with quantum simulators for ttH ($H \rightarrow \gamma\gamma$) analysis



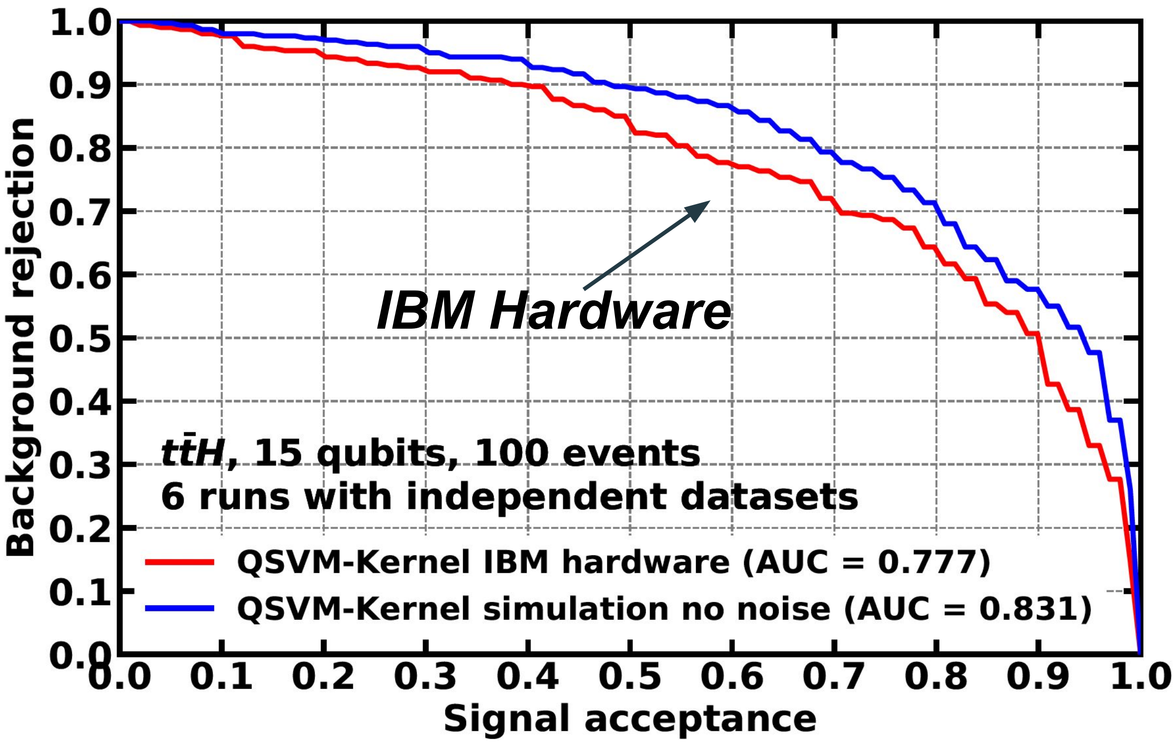
- **For 15 qubits, using ttH analysis dataset (20000 events), QSVM Kernel on simulator (red) achieves similar performances with classical SVM (blue) and classical BDT (green).**

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



- For 15 qubits, using ttH analysis dataset (20000 events), Google qsim simulator (red), IBM statevector simulator (blue), and Amazon local simulator (green) provide identical performances for QSVM Kernel method

Method 2: Employing QSVM Kernel with IBM hardware (ibmq_paris, a 27-qubit machine) for ttH ($H \rightarrow \gamma\gamma$) analysis



hardware AUC = 0.777

simulator AUC = 0.831

- **Using ttH 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

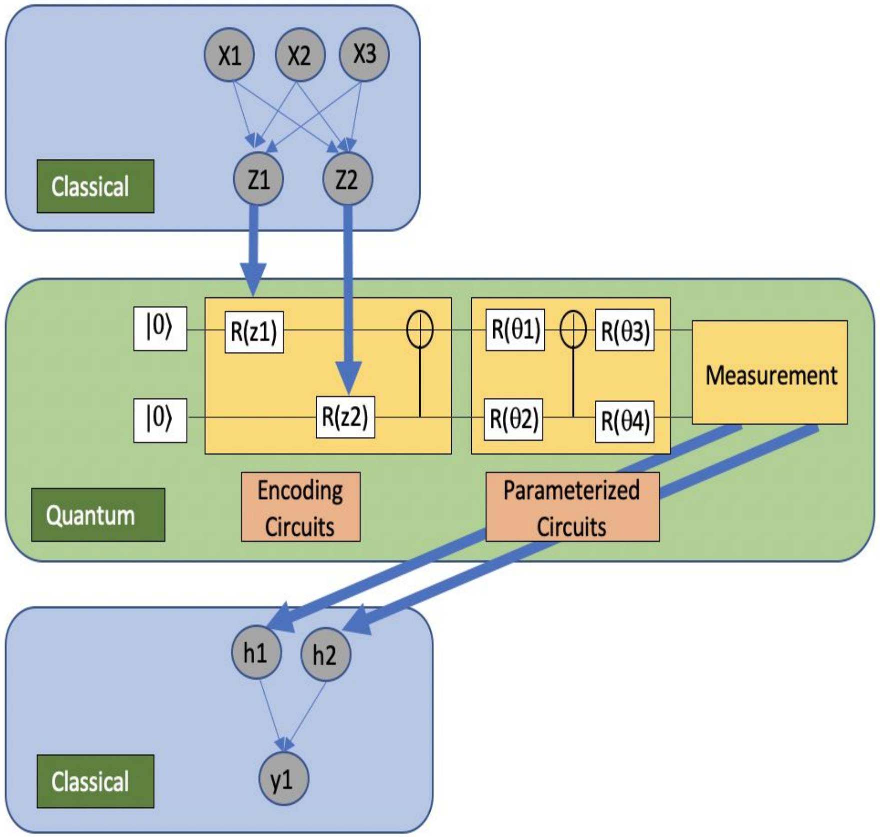
Employing Quantum Neural Network for ttH ($H \to \gamma\gamma$) analysis

Method 3: Quantum Neural Network (QNN)

- ***Quantum neural networks (QNNs): combining neural network algorithms and quantum computing***
  - ***Perform the computational intensive part of a neural network algorithm on a quantum computer with the aim of better efficiency and performance***
- ***Many QNN models have been recently studied in the field of quantum machine learning, for example, using Google Tensorflow quantum library and IBM Qiskit library***

Method 3: Hybrid Quantum Neural Network (QNN)

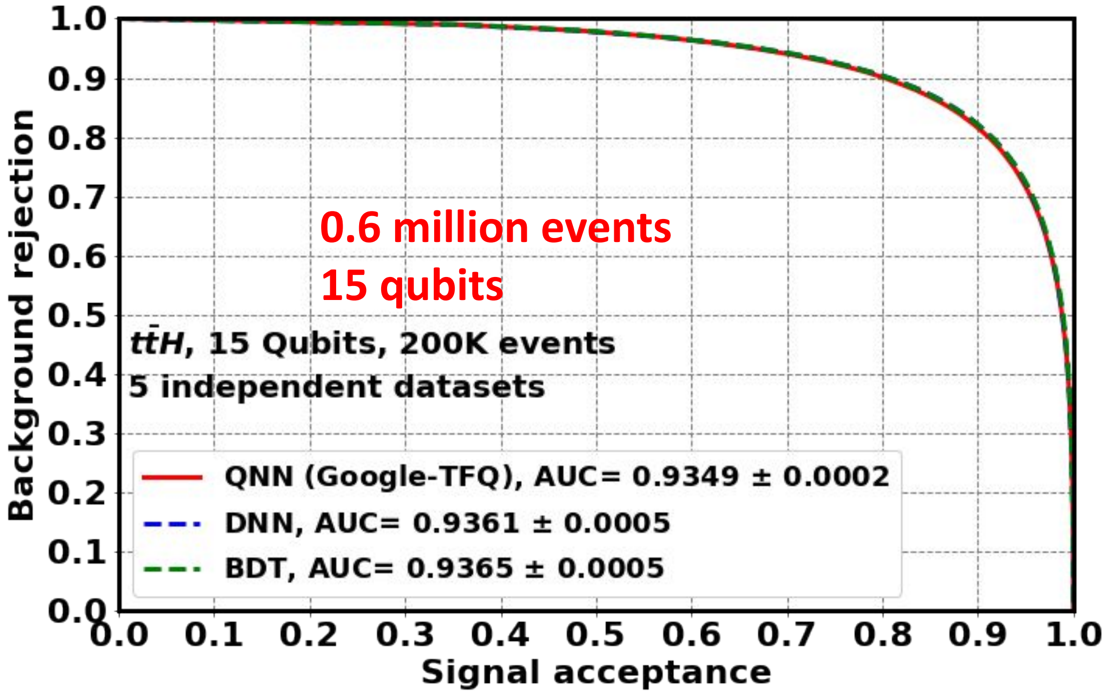
We have been exploring a hybrid QNN of three layers:



- ***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 ttH ($H \rightarrow \gamma\gamma$) analysis



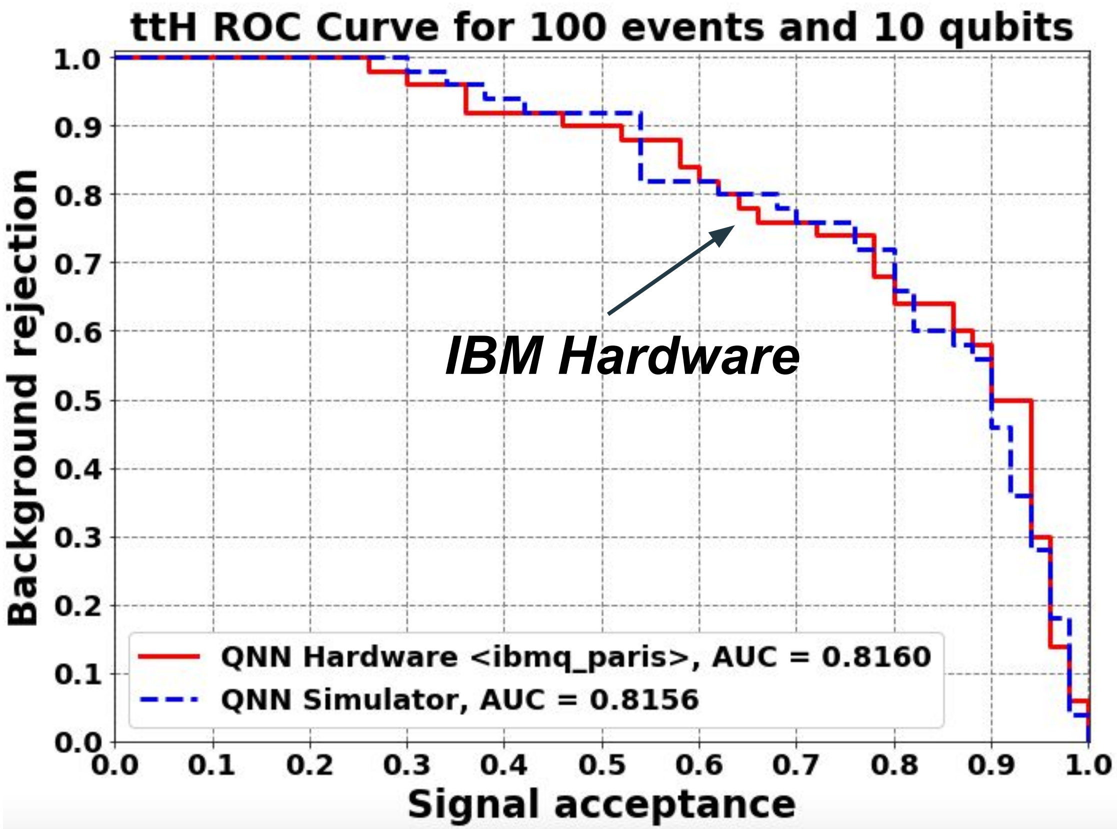
QNN AUC: 0.9349

DNN AUC: 0.9361

BDT AUC: 0.9365

- **Using the ttH analysis dataset with 0.6 million Delphes events 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 ttH ($H \to \gamma\gamma$) 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

Summary (part 1)

- **We have employed 3 methods of Quantum Machine Learning**

  - **Method 1: VQC-Variational Quantum Classifier**

    (J. Phys. G: Nucl. Part. Phys 48, 125003, 2021)
  - **Method 2: QSVM-Quantum Support Vector Machine Kernel method (Phys. Rev. Research 3, 033221, 2021)**
  - **Method 3: QNN-Quantum Neural Network (in progress)**

- **We have applied the three methods to two LHC HEP flagship analyses (ttH (H $\rightarrow \gamma\gamma$) and H $\rightarrow \mu\mu$) with Delphes simulation events.**

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

- Future developments:
  - We will investigate further and hopefully will see soon quantum machine learning outperforms classical machine learning, in particular, when more qubits are utilized
  - Furthermore, future quantum computers might offer speed ups in quantum machine learning which could be critical for the HEP community

* gate-based: computing is achieved by a sequence of quantum gates, as opposed to D-wave quantum annealers

Challenges ahead

- Difficulties at present:
  - Only 100 events are used in hardware jobs
    - Limited access time
  - Only 10-15 qubits are used in hardware jobs
    - So far circuit length and number of CNOT gates are limited in our present study.
- To use Quantum Computer Hardware for Machine Learning in future High-Luminosity LHC physics analyses, we need to extend our studies to larger event sample sizes and more qubits
- As of today, the maximal number of hardware qubits that I know of: 127 (IBM) and 54 (Google)
- To demonstrate that future Quantum Computers offer speed up in Quantum Machine Learning

OPPORTUNITIES

- I am confident that, in the near future,

  the quantum machine learning methods can demonstrate, in quantum simulation, the quantum advantage with a larger number of qubits (e.g. greater than 30 qubits).

  This is in the context of application to High Energy Physics data analysis.

OPPORTUNITIES

From the roadmap presented by IBM and Google, it is expected that quantum hardware in the future will reduce noise and achieve a performance close to noiseless quantum simulators. In addition, they are working hard to speed up the quantum hardware running time.

- **Specifically, industry roadmaps of quantum computer hardware project an exponential growth in the number of qubits, and that high-fidelity quantum computers will be available within the next 10 years.**

OPPORTUNITIES

From their roadmaps:

- IBM expects more than a thousand qubits (superconducting qubits) by 2023 and millions qubits soon after.
- IonQ expects to have quantum computers with more than one thousand algorithmic qubits (trapped Ion qubits) available with error correction by 2028.
- Google plans to build the error corrected quantum computers with more than one million qubits (superconducting qubits) by 2029.
- These roadmaps are evolving rapidly and the promised progress is impressive. With the large investments in quantum computing and fierce international competitions in technology, this expected opportunities are realistic.

OPPORTUNITIES

- "In conclusion, advanced quantum computers with large number of qubits, reduced noise and improved running time may outperform classical machine learning in both classification power and in speed. QML may well be a new computational paradigm for big data analyses in HEP. For this reason, the HEP community should stay aware of what is happening in quantum technologies – improvements in the hardware, software ecosystem and algorithms — to bring a quantum advantage to the HEP data challenge. Conversely, the development of solutions for unique HEP data challenges could also lead to contributions to the development of quantum technologies."

The above quotation from Sau Lan Wu and Shinjae Yoo is published in "Challenges and opportunities in quantum machine learning for high-energy physics": March 2022 issue of Nature Reviews Physics volume 4, issue 3 (2022).

New Project

We are working to exploit unsupervised machine learning for Anomaly Detection using quantum computers to search for new physics.

New Physics can be probed in the form of anomaly detection searches using AutoEncoder algorithm for example.