Quantum Computing

@CERN openlab

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OPENLAB JOINT R&D PROJECTS

High-bandwidth fabrics, accelerated platforms for data acquisition

Data Acquisition (LHCb, CMS, Dune, IT-CF)

Fast simulation, Data quality monitoring, anomaly detection, physics data reduction, benchmarking/scalability, systems biology and large-scale multi-disciplinary platforms

Data Analytics, Machine Learning (many)

Code modernization (EP-SFT, LHC Exp., OPL)

HPC, Cloud, Quantum

Predictive/proactive maintenance and operations

Control Systems (BE-ICS)

Cloud infra (IT-CM)

Cloud technology, containers, scalability

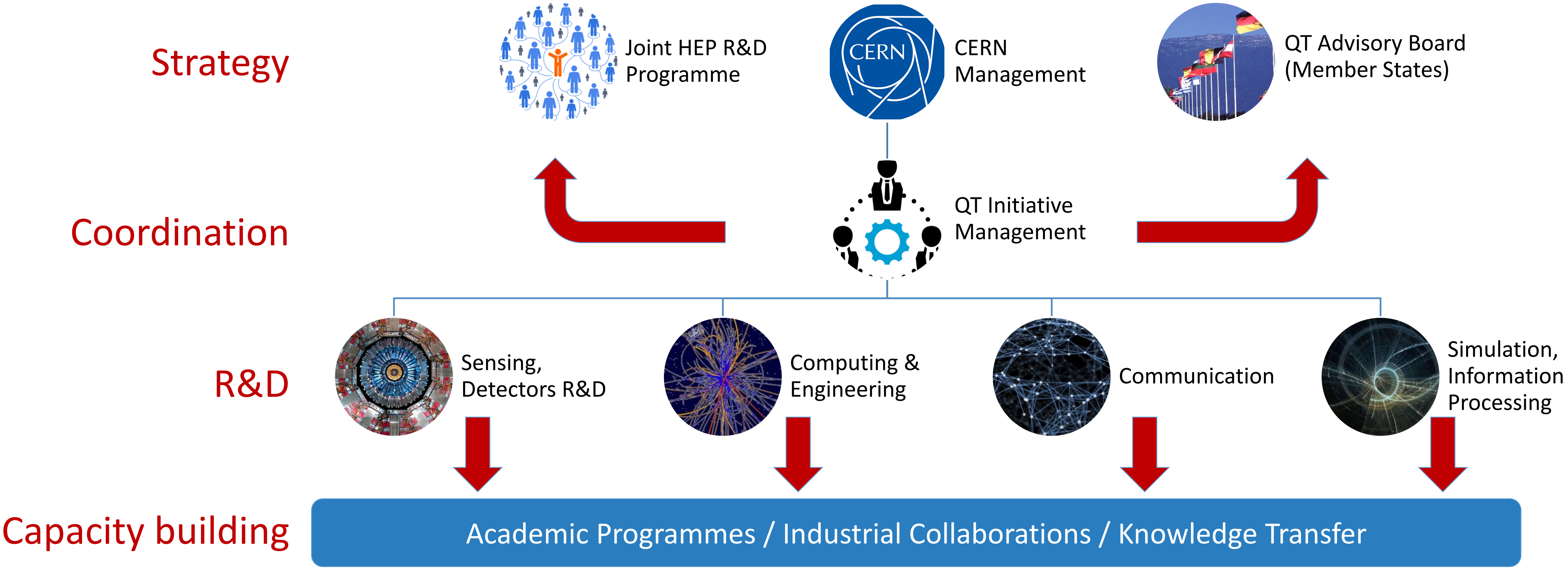
Software Defined Networks, Security

Networks (IT-CS)

Data Storage (IT-ST, IT-DB, EP-DT)

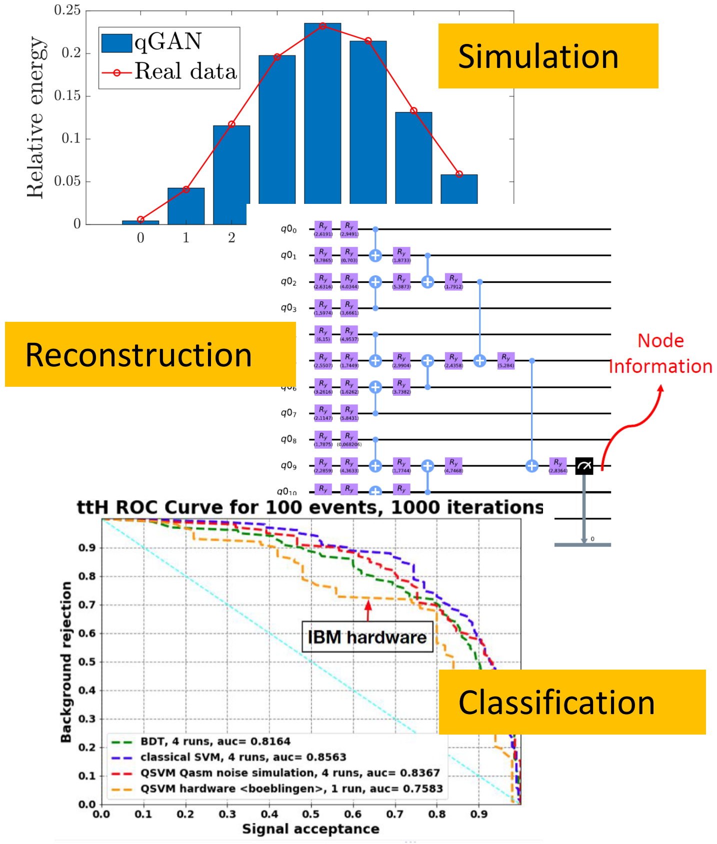
Storage architectures, scalability, monitoring

CERN Quantum Technology Initiative



Many pilot projects already started as part of the **CERN openlab quantum** programme (https://openlab.cern/quantum)

QC @ CERN openlab



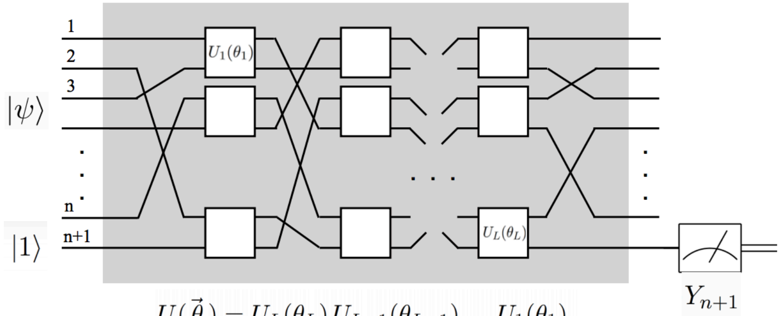
- Quantum **Generative Adversarial Networks** for detector simulation
- Quantum **Random Number Generators** tests and integration
- Quantum **Neural Networks** for particle trajectory reconstruction
- Quantum **Support Vector Machines** for signal/background classification (Higgs, SUSY,..)
- Workload optimization via quantum **Reinforcement Learning (D-Wave Quantum Annealer)**
- Quantum **Homomorphic Encryption**

Collaboration with institutes (DESY, U. Aachen, U.Tokyo, U. Wisconsin, METU, P. U. Bucharest, U. Oviedo, ..) and companies (IBM, Intel, CQC, ...)

Quantum Machine Learning

- QML introduces quantum algorithms as part of a larger implementation
  - **Fully quantum** or **hybrid** classical-quantum
  - Quantum or Classical **input data**
- How do we represent **learning rules**?
  - Need **association rule** between NN activation patterns and pure quantum states
- How do we address **data loading**?
  - **Quantum state preparation**
  - Encode information into **amplitudes** of a quantum state
  - **Direct access** through qRAM ?
- **Advantage**?
  - **Representational** power
  - **Computational** complexity? **Sample** Complexity?

QNN as variational circuits



$$U(\vec{\theta}) = U_L(\theta_L)\,U_{L-1}(\theta_{L-1})\ldots U_1(\theta_1)$$

E. Farhi, H. Neven, arxiv1802.06002

Examples

Quantum **Support Vector Machines** for signal/background **classification**

Quantum **Generative Adversarial Networks** for detector **simulation**

Quantum **Graph Neural Networks** for particle trajectory **reconstruction**

NOT A OPENLAB PROJECT

Quantum Annealing for ML

First QA application to HEP

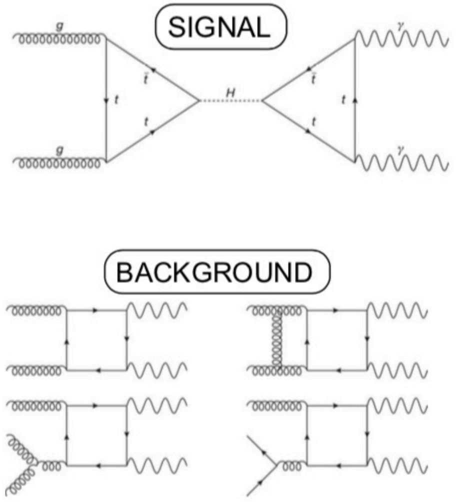
https://www.nature.com/articles/nature24047

Published: 19 October 2017

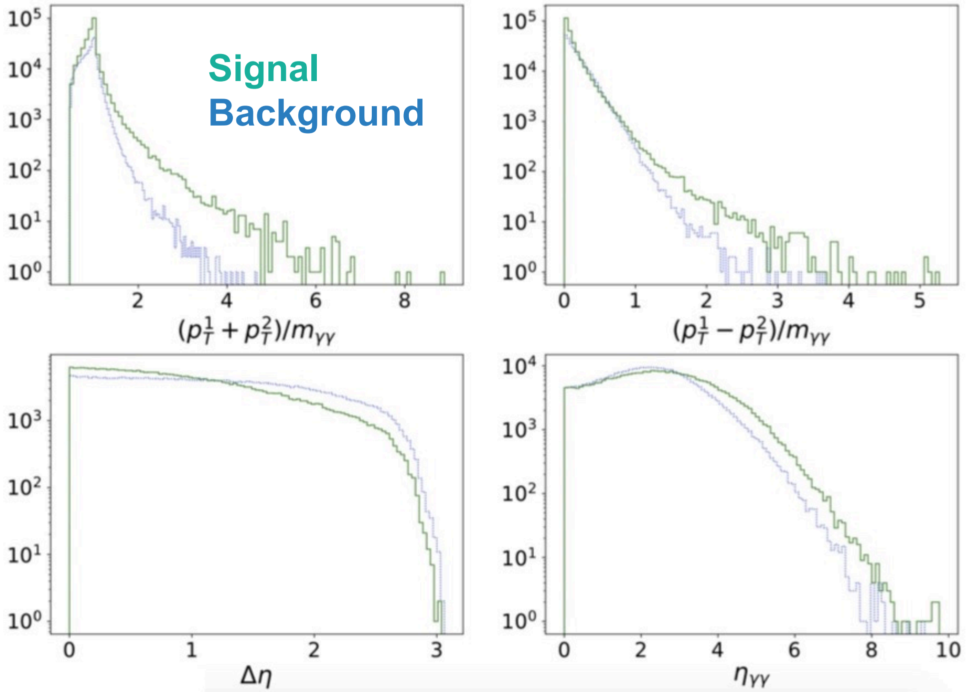
Solving a Higgs optimization problem with quantum annealing for machine learning

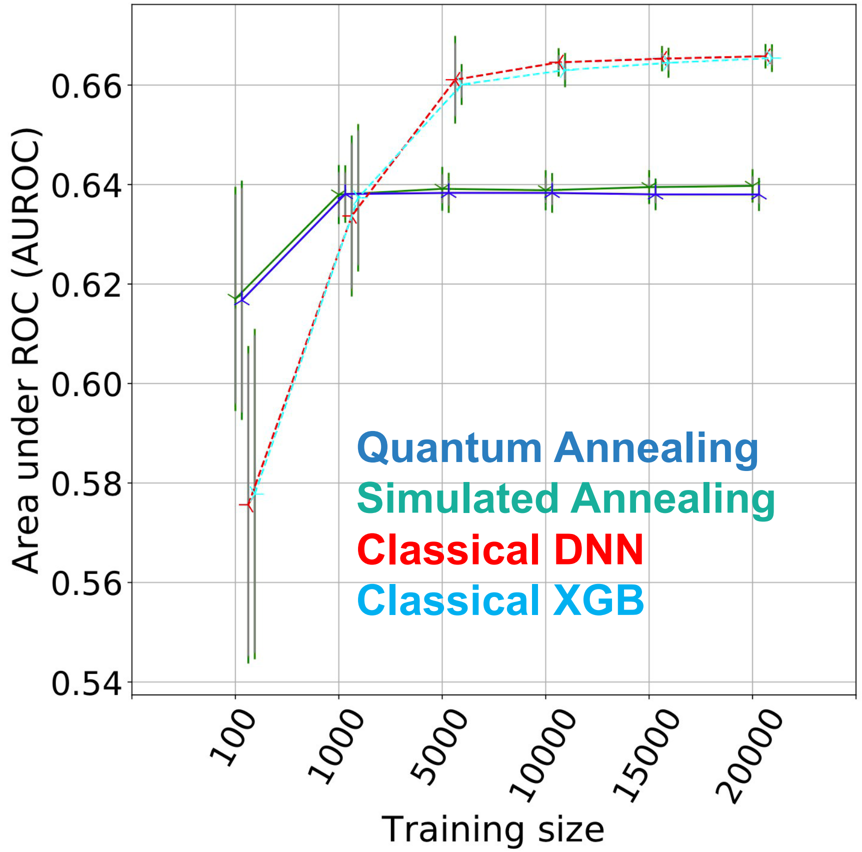
Alex Mott, Joshua Job, Jean-Roch Vlimant, Daniel Lidar & Maria Spiropulu

Nature **550**, 375–379(2017) | Cite this article



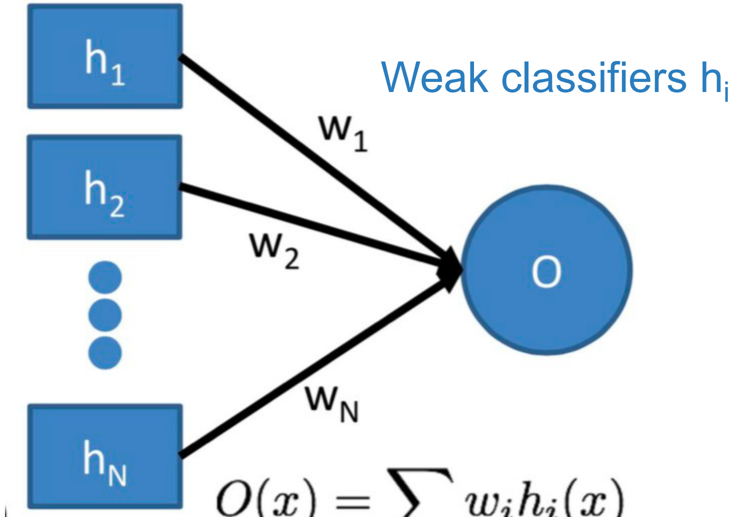
36 weak classifiers





Quantum Annealing

Evolution of a quantum system to a low T Gibbs state



$$O(x) = \sum_i w_i h_i(x)$$

Setup with trivial H_0 and evolve to target H_p in the ground state

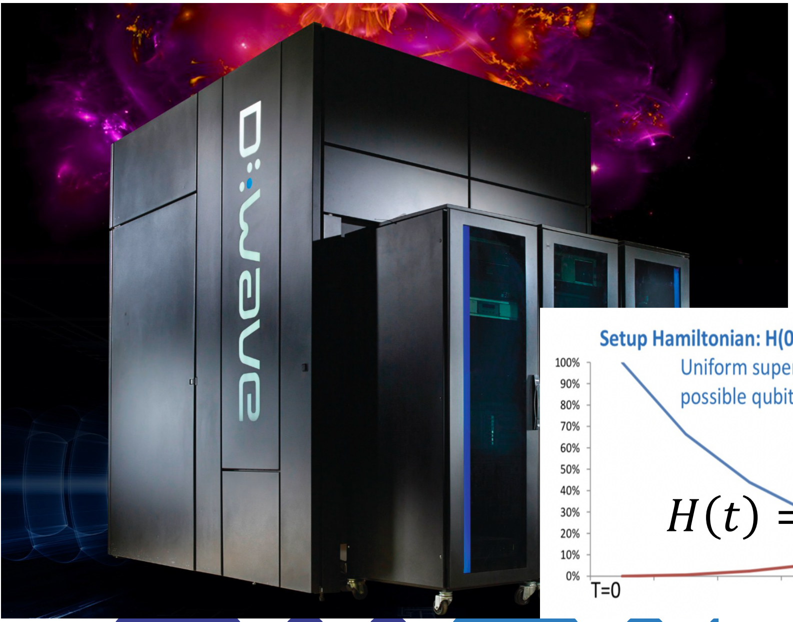
Adiabatic theorem : with a slow evolution of the system, the state stays in the ground state.

Total error over the training set:

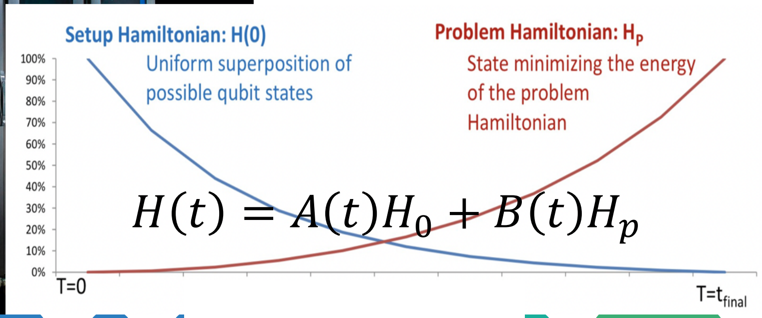
$$\delta(\vec{w}) \propto \sum_{i,j} C_{ij} w_i w_j + \sum_i (\lambda - 2C_{iy}) w_i$$

Quadratic
Unconstrained
Binary
Optimization

$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$



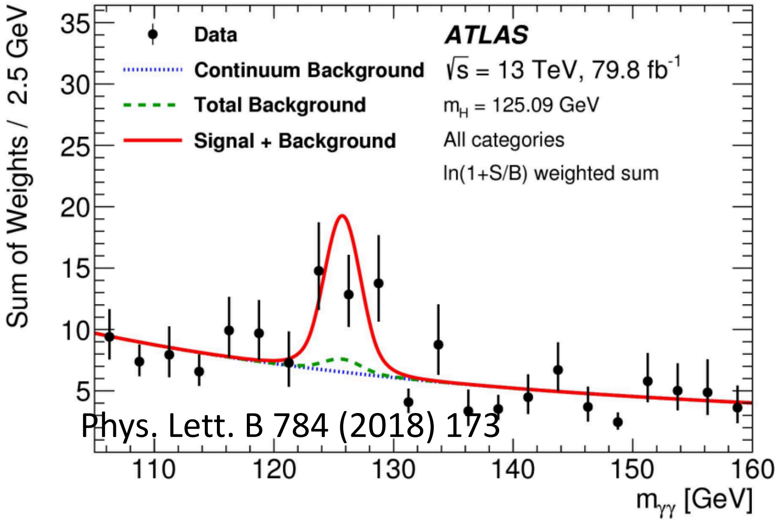
2017 D-wave 2X ™
1098 qubits
Operates at 15mK
Anneals in 5-20 µs



A Quantum Classifier

Quantum Support Vector Machines for Higgs classification

Prof. Sau Lan Wu and her team



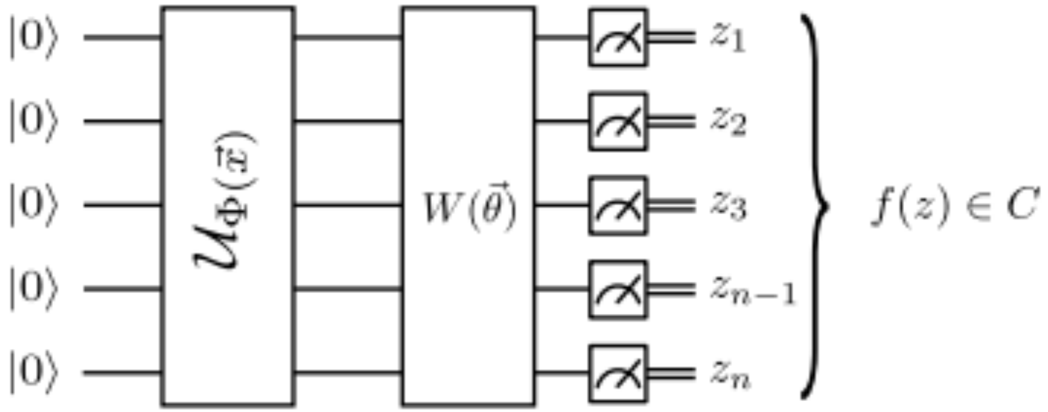
Phys. Lett. B 784 (2018) 173

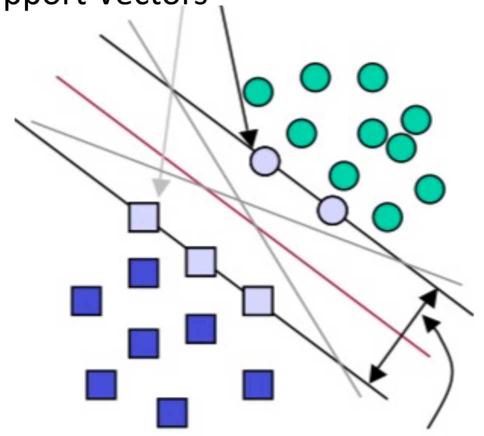
45 signal/background distinctive features

Define a quantum **SVM**

- Test different input **encoding**
  - Reduce number of input features using PCA :
  - 8,10,20 features (number of qubits)
  - Entanglement is used to encode relationships between features
- **Shallow variational classifier**
- Binary **measurement**

Simulate on **Qiskit**





CERN openlab

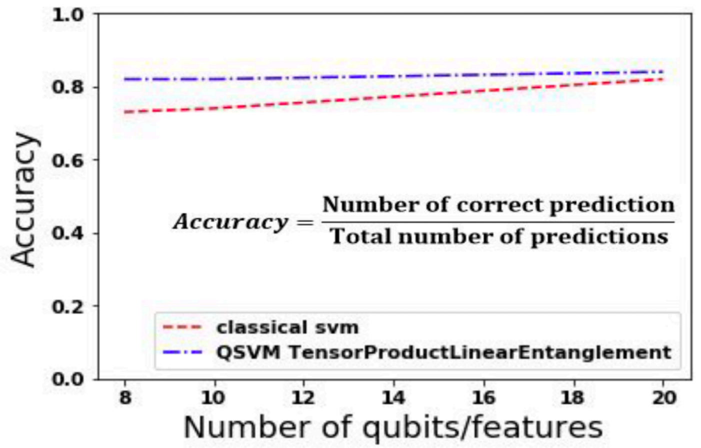
Quantum SVM

Quantum SVM for ttH($H \to \gamma\gamma$) classification

Prof. Sau Lan Wu and her team

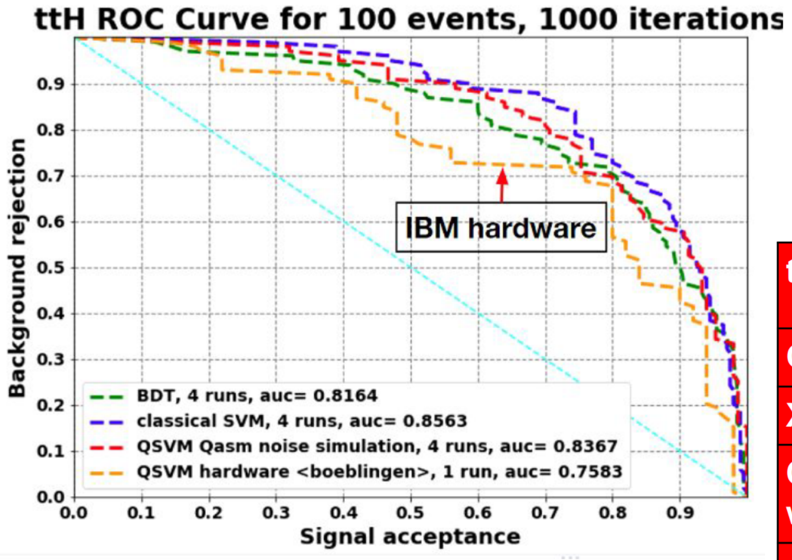
Comparison to BDT and classical SVM

- 100 training events, 100 test events, and 5 qubits
- 1000 iteration on IBM boeblingen



Running full training with quantum simulators requires **large computing resources**

- **Memory increases** with qubit, training events and complexity



ttH(H->$\gamma\gamma$) AUC	AUC
Classical SVM	0.856
XGBoost BDT	0.816
QSVM Simulation with Noise	0.837
QSVM Hardware	0.758

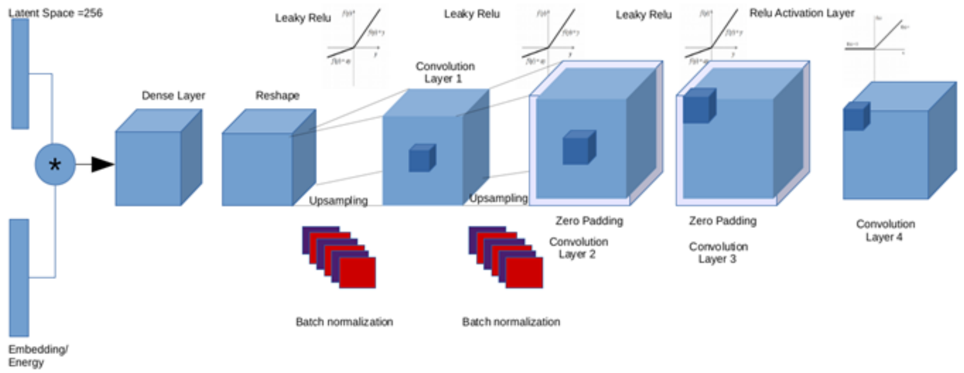
Quantum Generative Models

Su Yeon Chang

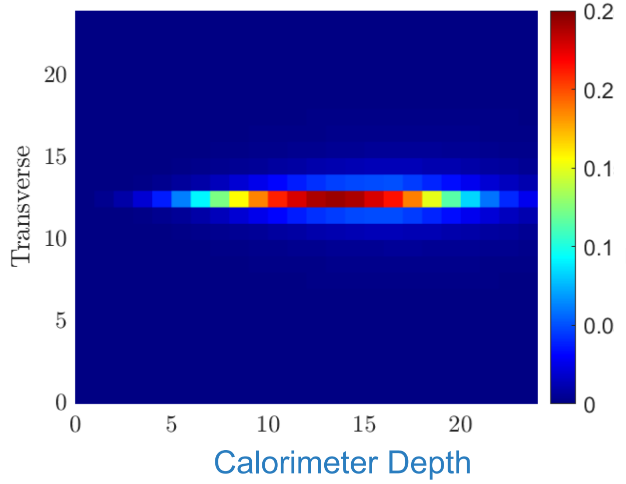
- Classical Generative Models can replace Monte Carlo simulation
  - **3DGAN: Generative Adversarial Networks** prototype for calorimeter simulation
  - Detector output interpreted as a 3D image.
- Quantum Generative Models might have **larger representational power**
- **Quantum GAN** investigations:
  - Down sample 3DGAN use case to **manageable number of pixels**
  - Use **compressed data representation** in quantum states.
    - **Qubits** or **Continuous Variables**
  - Different **hybrid** classical-quantum combinations

3DGAN generator

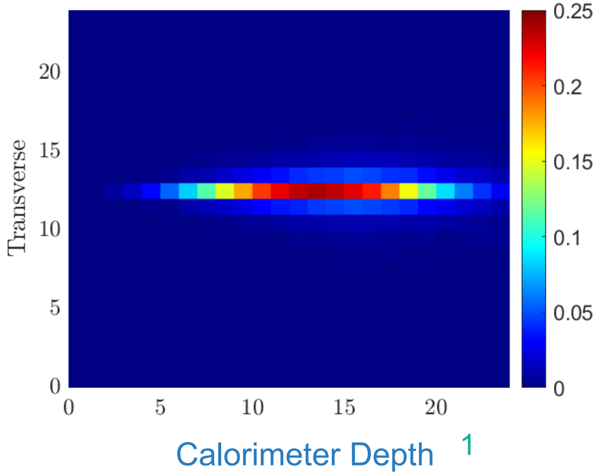
https://doi.org/10.1051/epjconf/201921402010



Real image



3DGAN output



Su Yeon Chang

Hybrid Classical-Quantum GAN

IBM qGAN can load probability distributions in quantum states

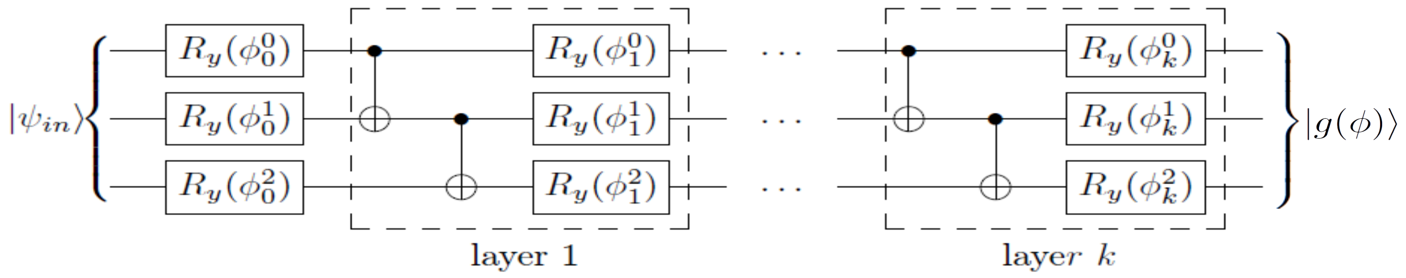
Simplify dataset: extract 1D energy profiles from 3DGAN images

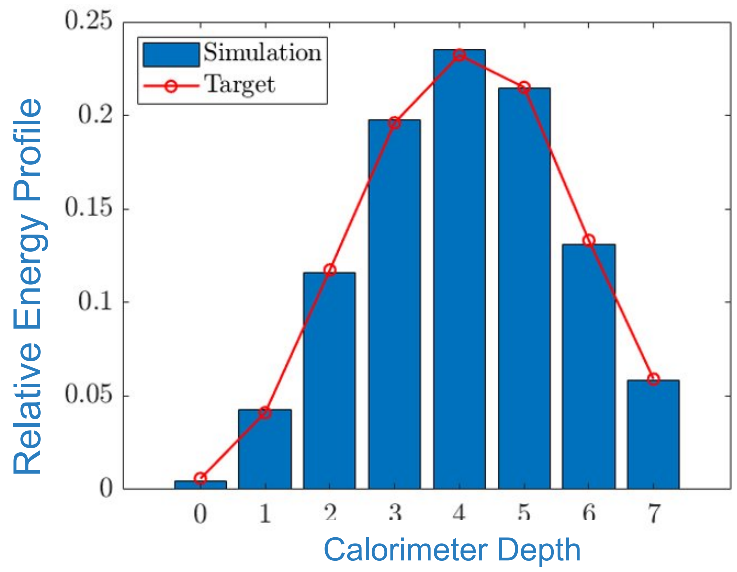
- 2^n classical pixels expressed by n qubits
- Probability of getting state $|k\rangle$ = (Relative) Energy at pixel k

Train a hybrid classical-quantum GAN to generate **few-pixels image**

- **Classical Discriminator (pyTorch):** 512 nodes + Leaky ReLU → 216 nodes + Leaky ReLU → single-node + sigmoid
- **Quantum Generator (Qiskit): 3 R_y layers**

https://doi.org/10.1038/s41534-019-0223-2





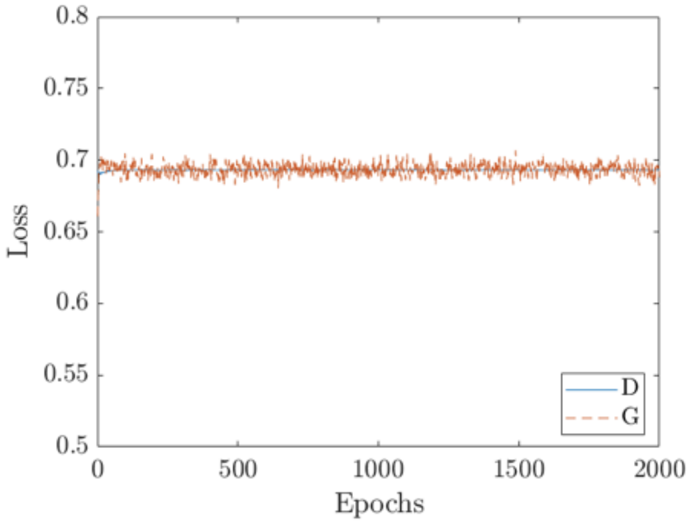
qGAN for single electron in a electromagnetic calorimeter

EPFL CERN openlab
Su Yeon Chang

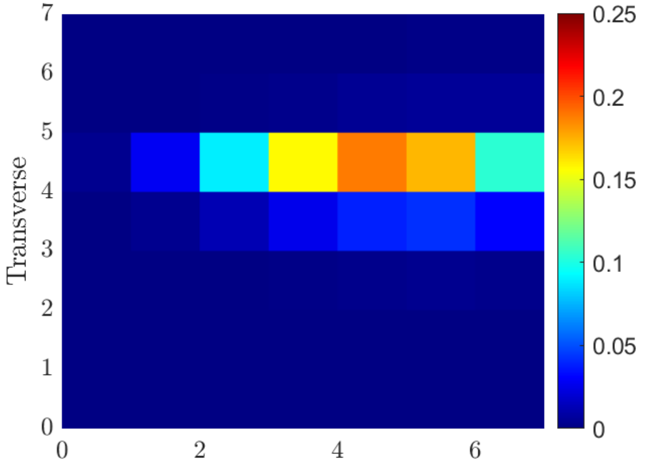
Low resolution 2D energy profile

Increase generator and discriminator depth (6 qubits – 36 pixels)
  Realistic 2D images
  Stable training losses

IBM qGAN is not a real generative model
  It uses the adversarial training approach to **embed** image probability distribution in a quantum circuit
Need a way to sample single images

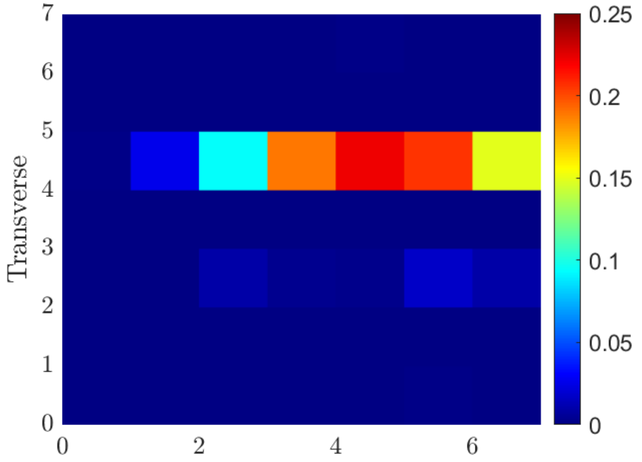


Real image



Calorimeter Depth

qGAN image



Calorimeter Depth

Su Yeon Chang

Extending the qGAN model

Collaboration with Cambridge Quantum Computing

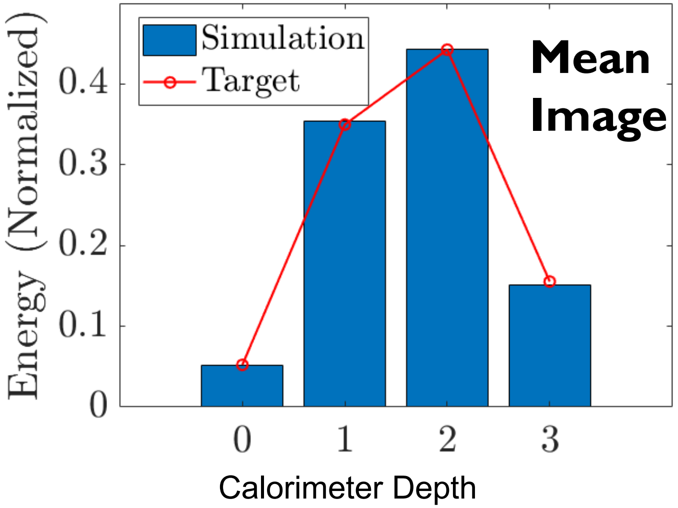
WORK IN PROGRESS

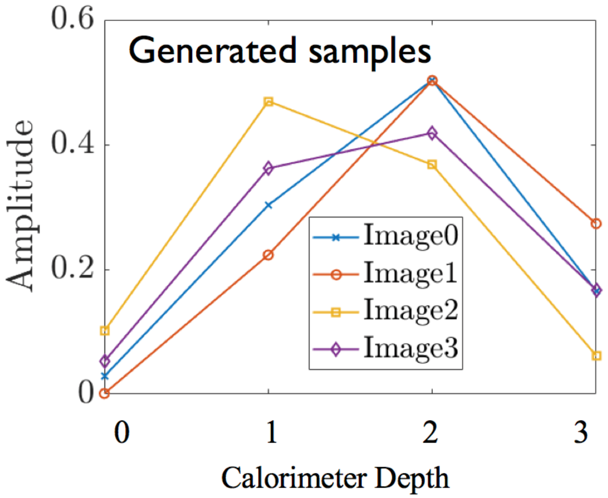
Two-steps quantum generator to learn the average distribution and sample images from it

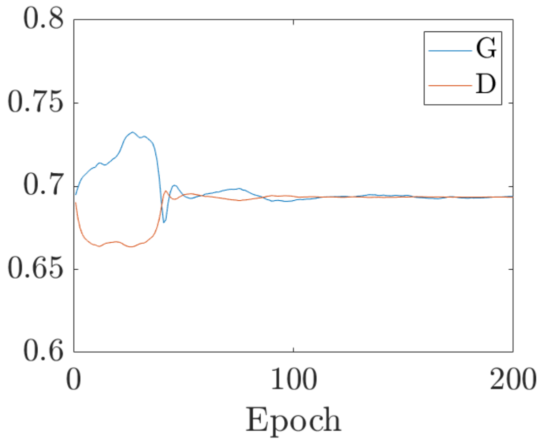
- Ry variational form implemented using **qiskit & t|ket**
- Uniform parameter initialization
- AMSGRAD optimizer with lr = 10^{-4}, lr2 = 10^{-3}

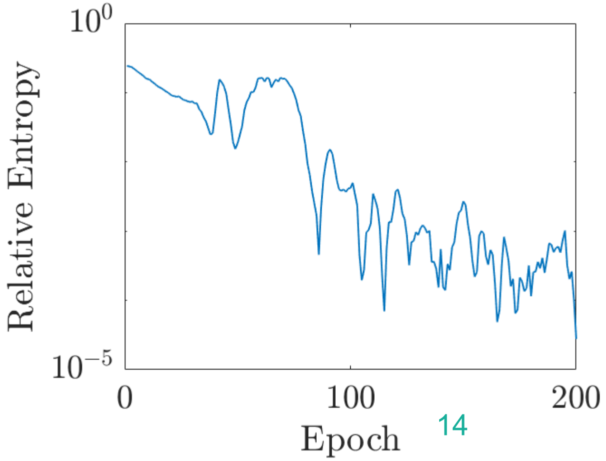
Classical discriminator (pyTorch) 4 nodes → 512 nodes → 256 nodes → 1 node

- Leaky ReLu between hidden layers + sigmoid
- AMSGRAD optimizer + Gradient penalty for stability and convergence







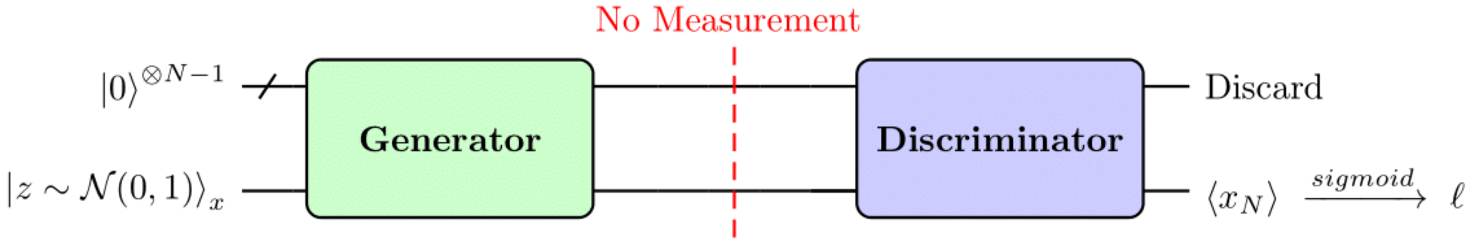


Continuous Variable qGAN

Alternative concept based on optical systems

- Information encoded in continuous physics observables (ex : strength of EM field)
- Information-carrying units: **qumodes** $|\psi\rangle = \exp(-iHt)\,|0\rangle = \int dx\, \psi(x)|x\rangle dx = \sum_{n=0}^{\infty} \langle n|\psi\rangle |n\rangle$

Fully Quantum model :



Hybrid model :

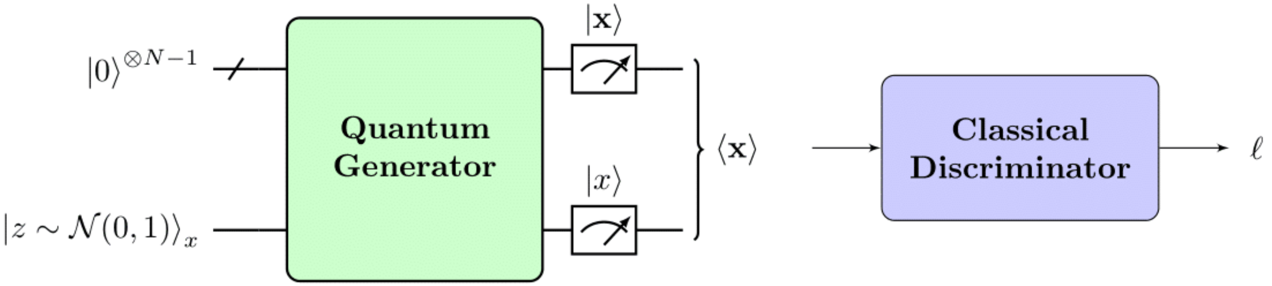
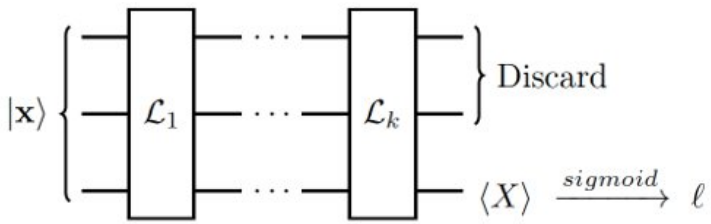


Image data encoded as a displaced state $|\boldsymbol{x}\rangle = \otimes_{i=1}^{N} |x_i\rangle = \otimes_{i=1}^{N} D_i(x_i)|0\rangle$

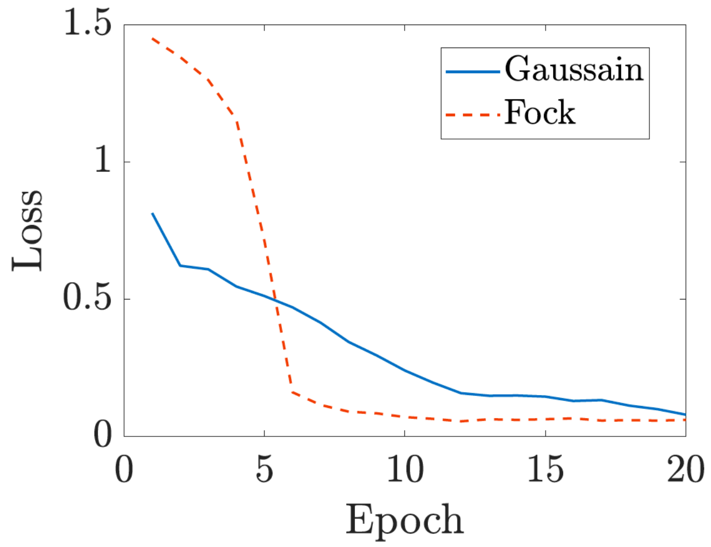
CV classifier

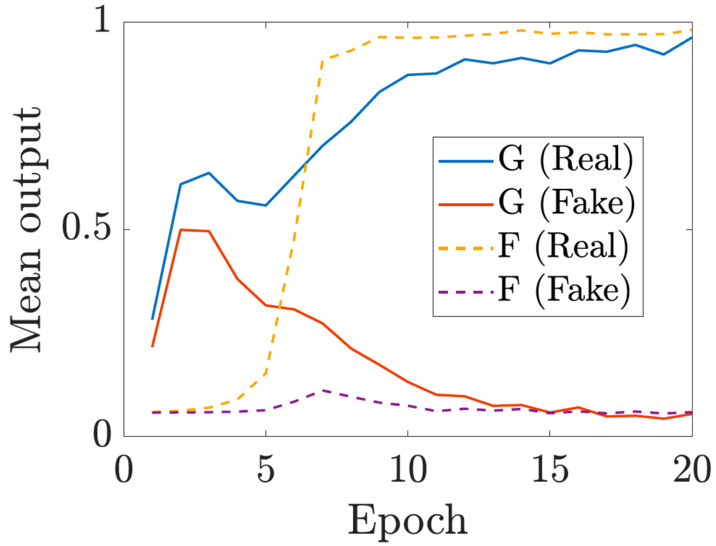
Test quantum discriminator network n=3 depth =3

StrawberryFields for network implementation.
Pennylane for autodifferentiation



Compare 1D energy profile to flat distribution





Fock

Prediction outcome

actual value	p	n
p′	1.0	0.0
n′	0.036	0.964

Gaussian

Prediction outcome

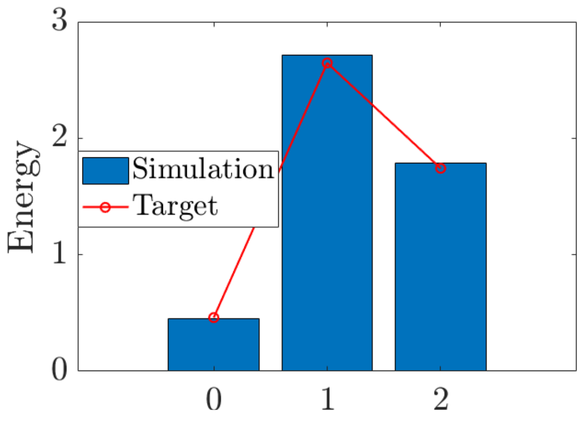
actual value	p	n
p′	0.984	0.016
n′	0.039	0.961

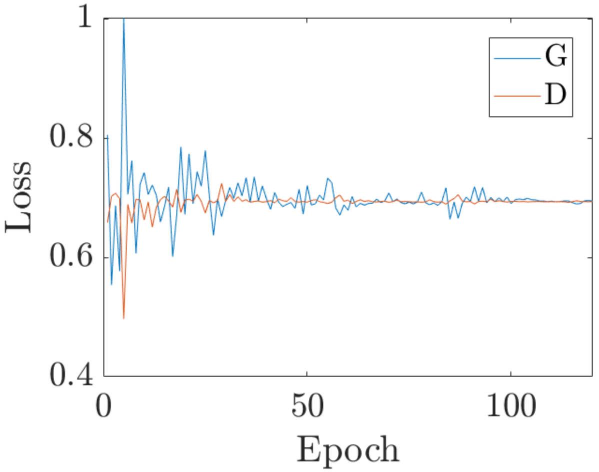
https://doi.org/10.1103/PhysRevLett.82.1784

cvGAN preliminary results

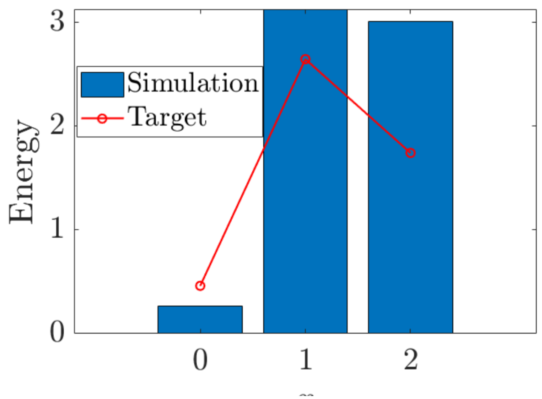
WORK IN PROGRESS

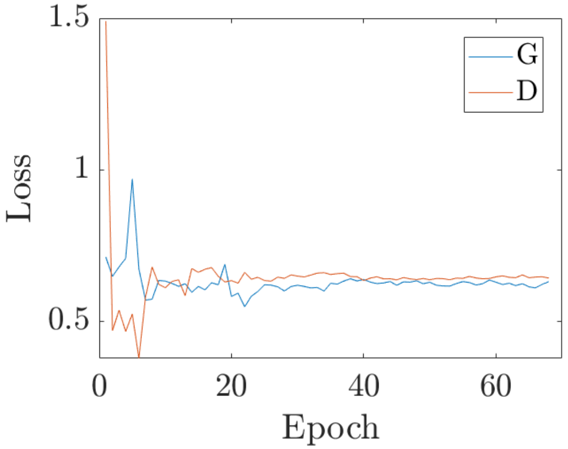
Hybrid



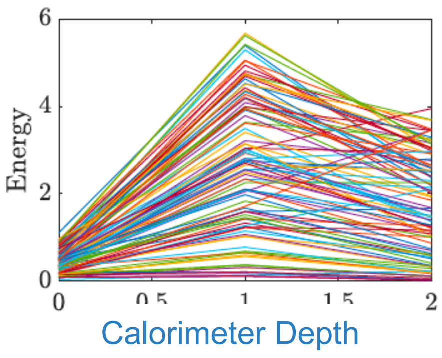


Fully Quantum

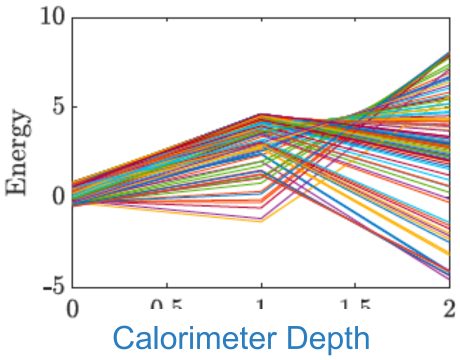




Real



Fully quantum qGAN



Fully quantum approach doesn't fully converge

- Use **non-linear activation** function (kerr gate) for the generator
- Generator is probably not strong enough
  - Try image clustering approach

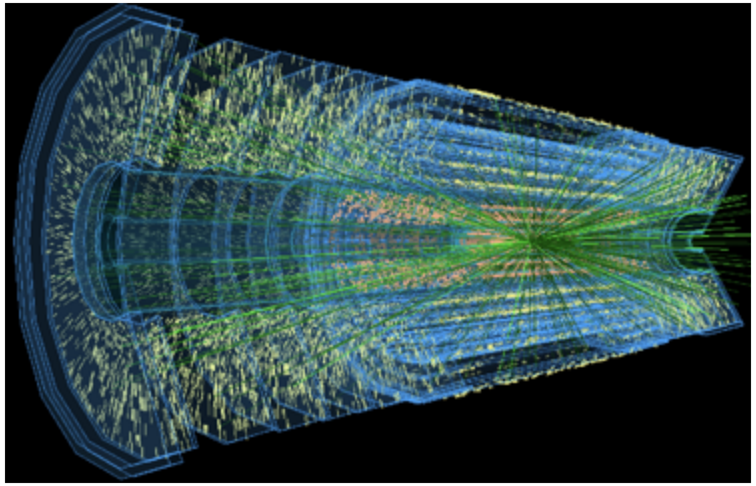
Training process is time-consuming and limited by **computing power**

- multiprocessing with 50 cores yields
  - **160 min/epoch (quantum)**
  - **80 min/epoch (hybrid)**

Charged particle tracking

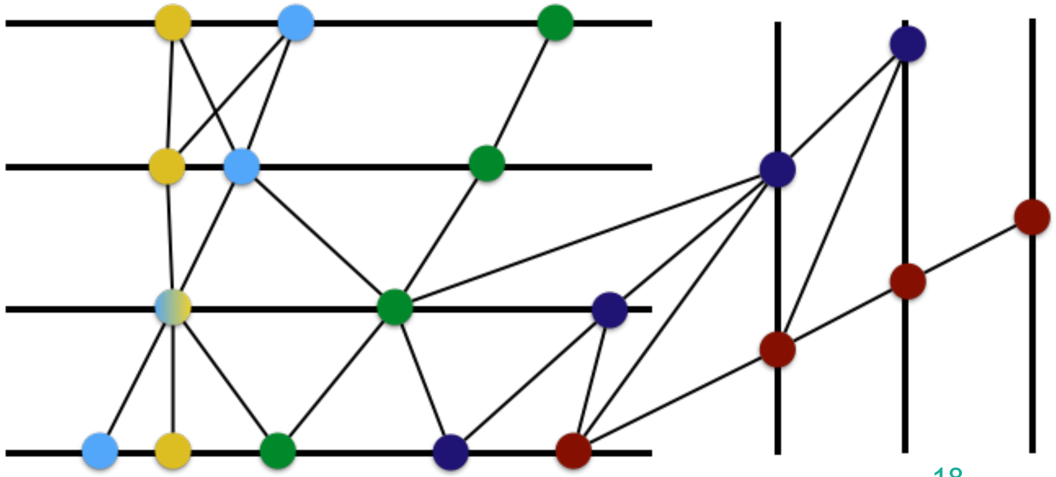
Hep.TrkX project introduces **Graph Neural Networks** for particle trajectory reconstruction

- Data as a **graph of connected hits**
- Connect plausibly-related hits using geometric constraints
- Full event embedding requires **large graphs** (~10^5 nodes)



HepTrkX GNN is a cascade of **Input**, **Edge** and **Node** Networks

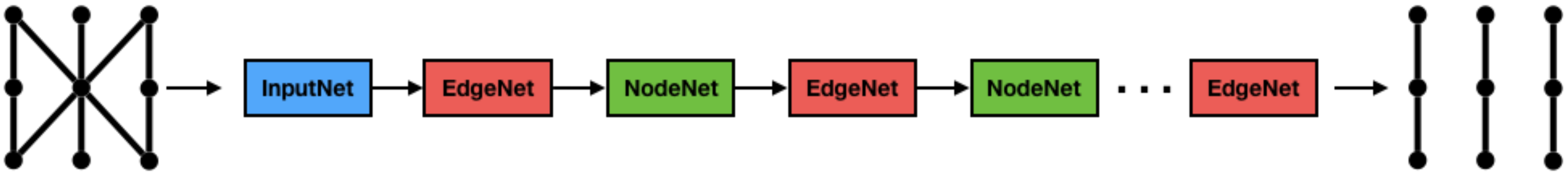
- **Edge network** outputs edge features, using the start and end nodes
- **Node network** classifies nodes using all connected nodes fewatures on the previous and next layers

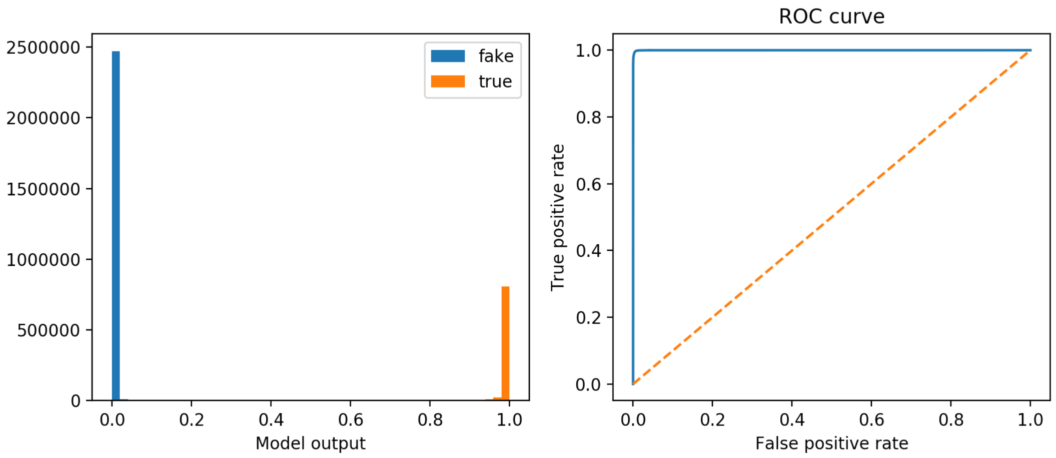


arxiv:1810.06111

First results at CHEP 2019 [arxiv:2003.08126](https://arxiv.org/abs/2003.08126)

GNN for particle tracking

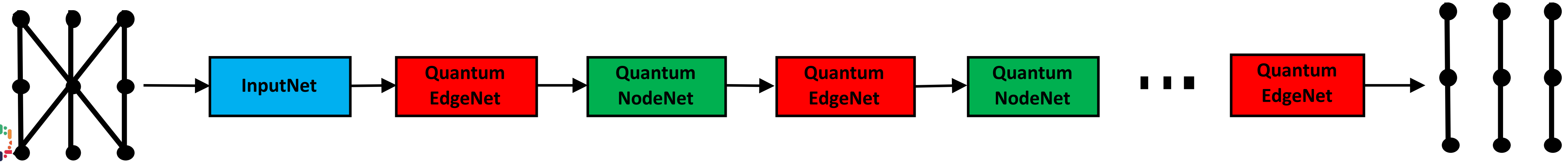




HEP.TrkX GNN Scores:

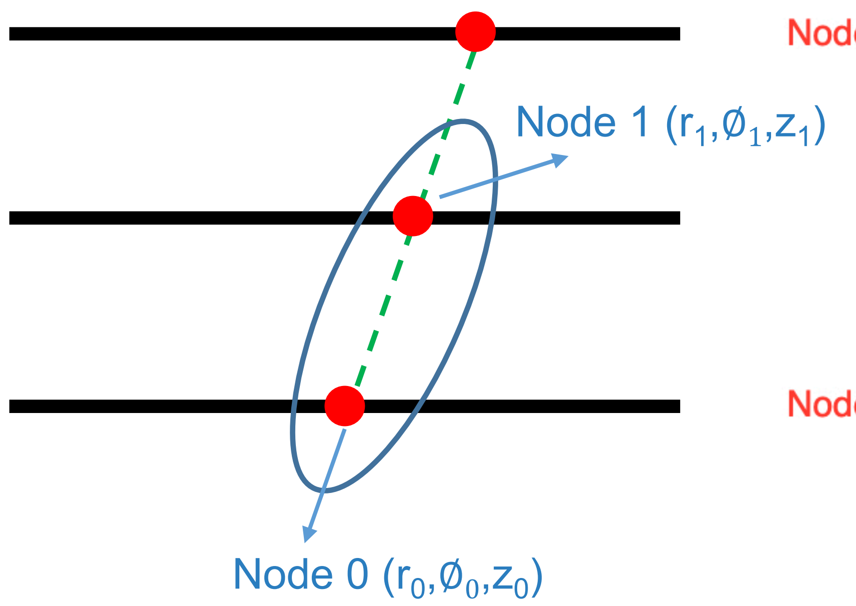
- Purity: 99.5%
- Efficiency: 98.7%
- Overall Accuracy: 99.5% with 0.5 threshold

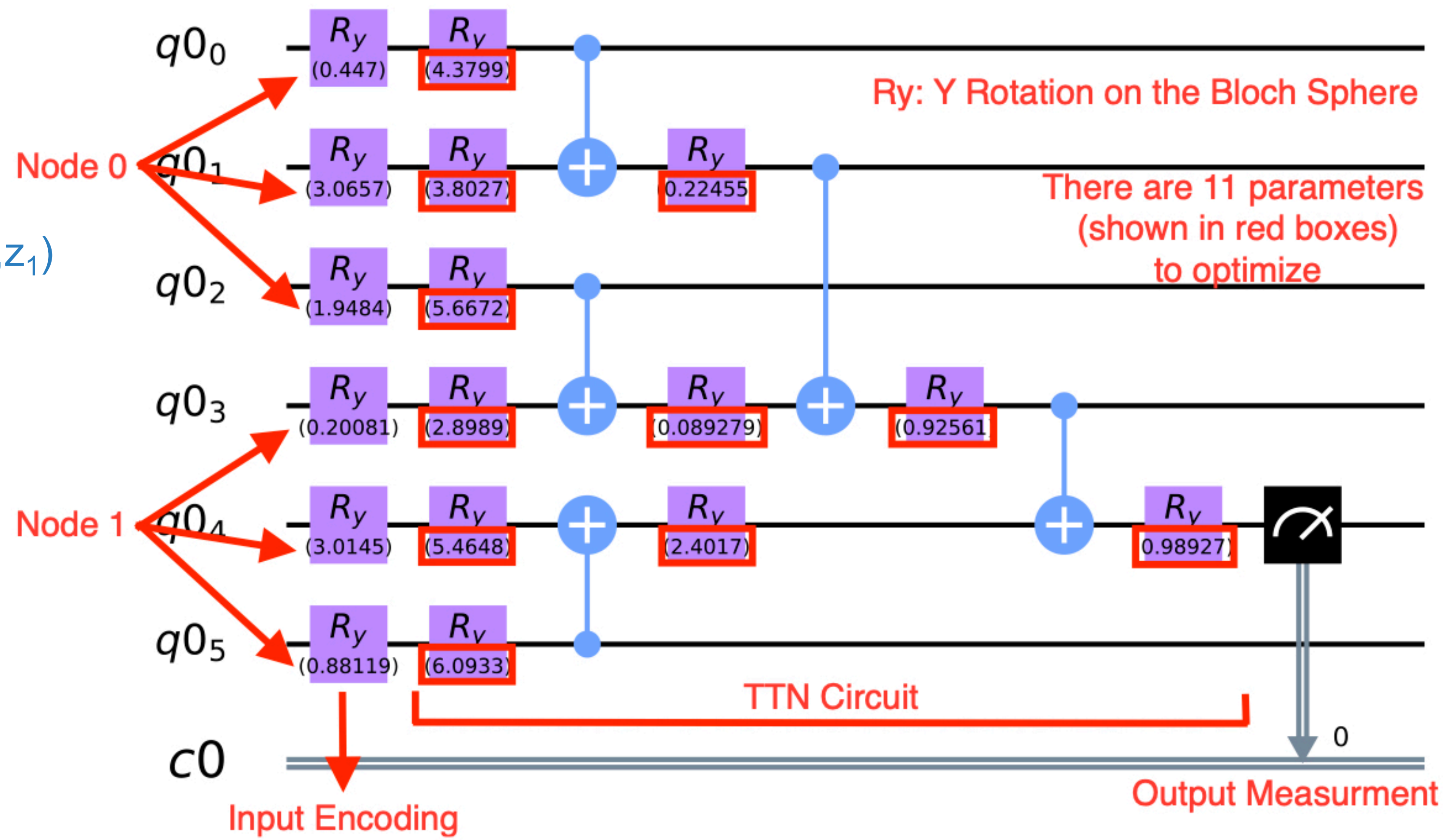
Quantum: Gate Level implementation



A Quantum Classifier

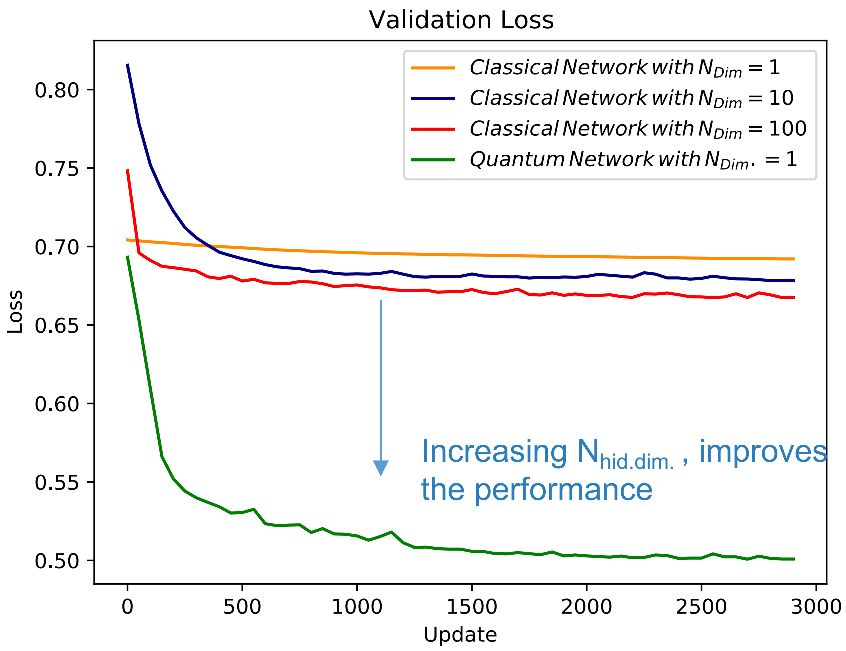
Edge and Node NN as Tree Tensor Networks

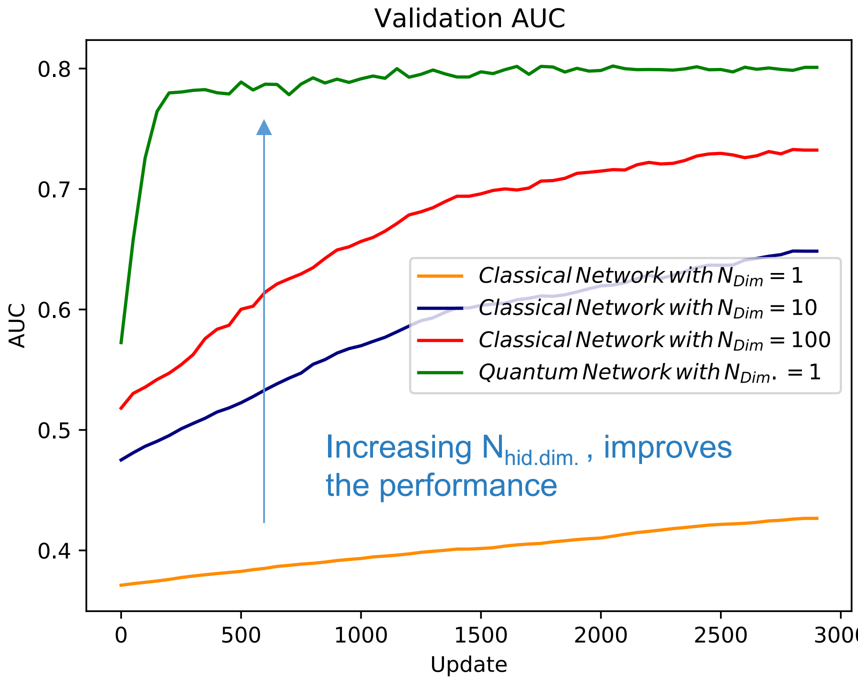




Training Results of the QGNN

Comparison to Simple Classical Networks (2 epochs)





Training set: 1400 subgraphs, **Validation set**: 200 subgraphs,
ADAM optimiser, binary cross entropy, lr = 0.01, shots =1000. **Hidden Dimension Size = 1**.
Classical Networks have x100 learning rate.

Simple experiments with Classical Networks show the potential for the Quantum Network.

Summary

CERN Quantum Technology Initiative established

- **Assess the potential of QC** in the time scale of the High Luminosity LHC runs and beyond
- **Build skills** for future programmes
- Provide a thematic **HEP focus** for international collaborations

CERN openlab is investigating opportunities in QC and across QC and other relevant fields (AI, HPC)

- Foster **collaborations between scientists and industry**
- Major focus on **education and skills development**

Initial **results are very exciting**

- **Quantum Machine Learning** particularly promising

Classical computational resources for simulation are an issue

- Easy access to a full hardware+software stack can highly increase productivity

Thanks!

https://openlab.cern/quantum