Quantum Computing at CERN

QUANTUM
TECHNOLOGY
INITIATIVE

Sofia Vallecorsa
AI and Quantum Research - CERN openlab
CERN

CERN QTI and its Roadmap

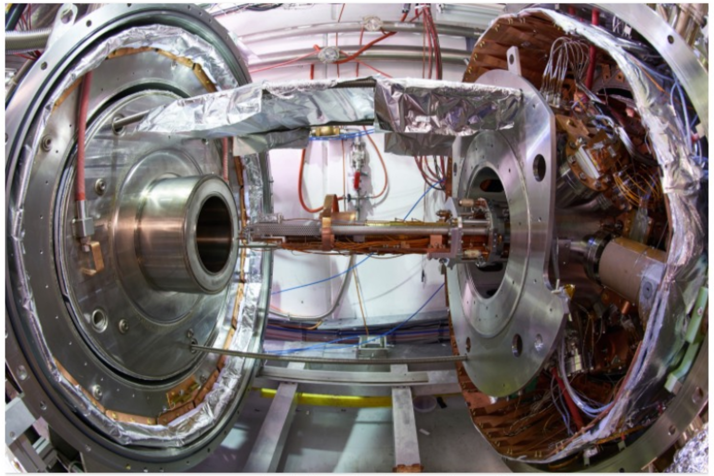
CERN established the QTI in 2020

Voir en français

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By Matthew Chalmers



The AEgIS 1T antimatter trap stack. CERN's AEgIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

- Roadmap in 2021, after a process of iterative consultations
- Publicly available in Zenodo, it has been accessed more than 4,300 times

T1 - Scientific and Technical Development and Capacity Building

T2 - Co-development

APPLICATIONS | NEWS

CERN unveils roadmap for quantum technology

4 November 2021

QUANTUM TECHNOLOGY INITIATIVE

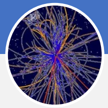
Credit: CERN

T3 - Community Building

T4 - Integration with national and international initiatives and programmes

https://doi.org/10.5281/zenodo.5553774

Scientific Objectives



- Assess the **areas of potential quantum advantage** in HEP (QML, classification, anomaly detection, tracking)
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

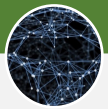
Computing & Algorithms

- Identify and develop techniques for **quantum simulation** in collider physics, QCD, cosmology within and beyond the SM
- Co-develop quantum computing and sensing approaches by providing **theoretical foundations** to the identifications of the areas of interest

Simulation & Theory

- Develop and promote **expertise in quantum sensing** in low- and high-energy physics applications
- Develop quantum sensing approaches with emphasis on **low-energy particle physics measurements**
- Assess **novel technologies and materials** for HEP applications

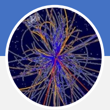
Sensing, Metrology & Materials



- **Co-develop CERN technologies relevant to quantum infrastructures** (time synch, frequency distribution, lasers)
- Contribute to the **deployment and validation of quantum infrastructures**
- Assess requirements and **impact of quantum communication on computing applications** (security, privacy)

Communications & Networks

Scientific Objectives



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Computing & Algorithms

Assess the **areas of potential quantum advantage** in HEP applications (QML, classification, anomaly detection, tracking)

QC Algorithms

- Quantum Machine Learning algorithms are a primary candidate for investigation
  - Increasing use of such techniques in many computing and data analysis flows
  - Can be built as **hybrid models** where quantum computers act as accelerators where classic computing is not computationally efficient
- Classification, pattern recognition, anomaly detection
- Clustering, optimisation
- Efficient data handling is a challenge
  - Data encoding or reduction is required for practical use of NISQ devices

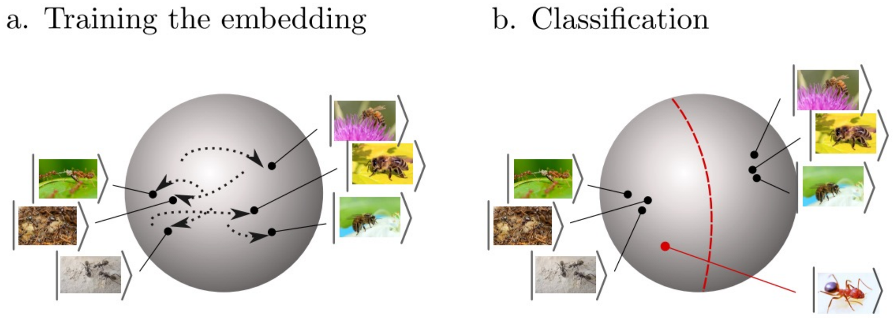
QML in practice…

How do we **represent classical data** in quantum states?

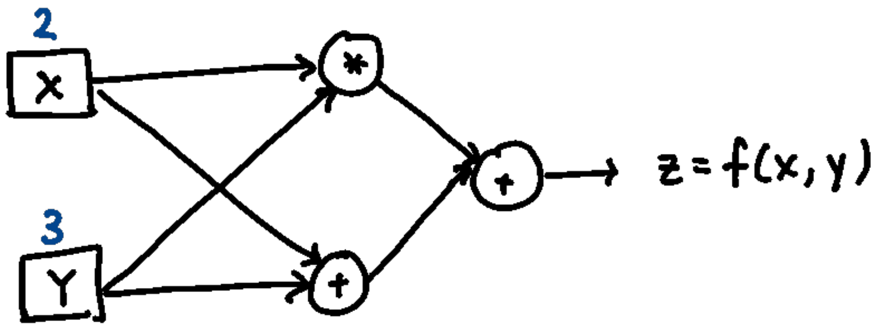
How do we introduce **non-linearities** in quantum circuits?

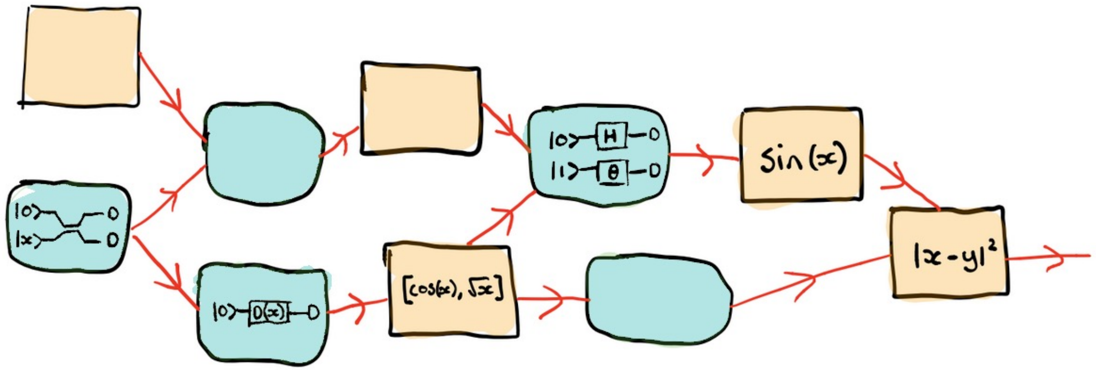
SGD-based **optimisation**?

Back-propagation and **automatic differentiation**



M. Schuld et al., arXiv: 2001.03622v2



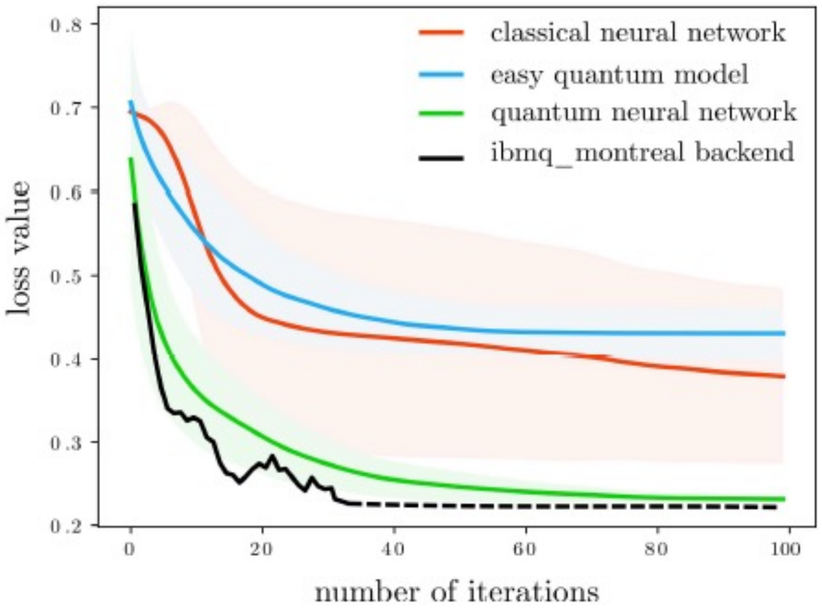


Images from pennylane.ai tutorial

Mitarai et al. (2018)
Schuld et al. (2018)

Quantum Advantage for QML?

A. Abbas *et al.*, arxiv:2011.00027



Advantage definition

- Runtime speedup
- Sample complexity
- Representational power

Practical implementation vs asymptotic complexity

- Data embedding
- NISQ vs ideal quantum devices
- Realistic applications

Performance metrics

Classical vs Quantum Data

A change of paradigm in the study of QML algorithms could reflect in interesting insights in classical models as well

see recent work by M. Schuld and N. Killoran (arxiv:2203.01340)

Example QML projects

CERN openlab

Quantum Classifiers for Higgs boson identification

arXiv:2104.07692

Quantum Tree Tensor Networks for particle trajectory reconstruction

arXiv:2007.06868, arXiv:2012.01379, arXiv:2109.12636

Hybrid quantum-classical tracking hits embedding

EPJ Web of Conferences (Vol. 251, p. 03065)

Quantum Generative Adversarial Networks for detector simulation

arXiv:2103.15470, arXiv:2101.11132, arXiv:2203.01007

Quantum Born Machines for event generation

ACAT2021

Quantum Boltzmann Machines for beam optimization in accelerators

BQiT 2021

Quantum algorithms for anomaly detection

Generative Modelling

The task of **generalising from a finite set of samples** drawn from a data set.

- Learn the underlying probability distribution
- Generate new samples from the learned distribution

Classical Generative Models can simulate detector output and replace Monte Carlo

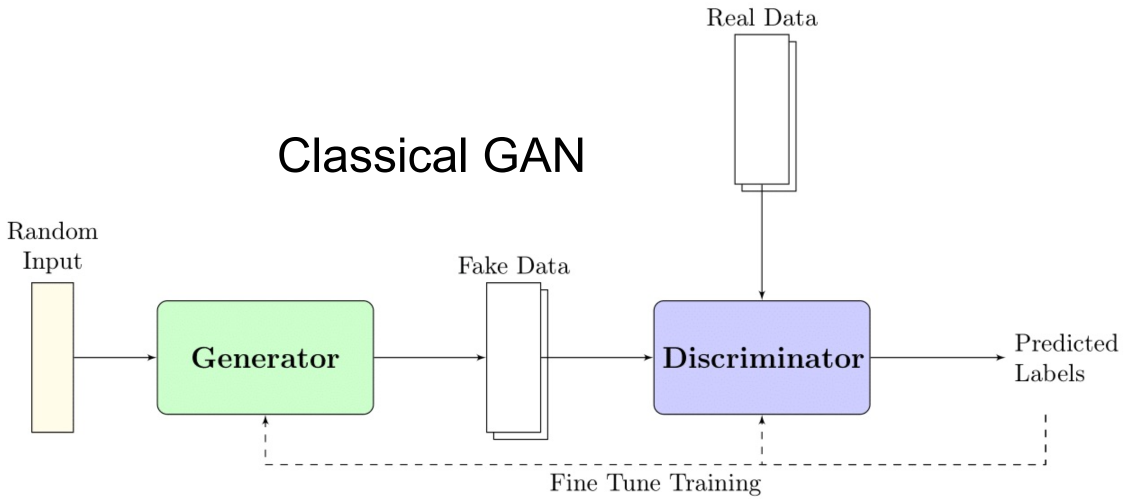
Explore quantum models:

- **Compressed data representation** in quantum states
- **Help understand convergence and generalization?**
- **Support space** of the learned distribution?

Examples include **quantum implementations** of

- **Generative Adversarial Networks (GAN)**
- **Born Machines**
- Boltzman Machines
- Auto-Encoders

Classical GAN



Quantum generation of energy profiles

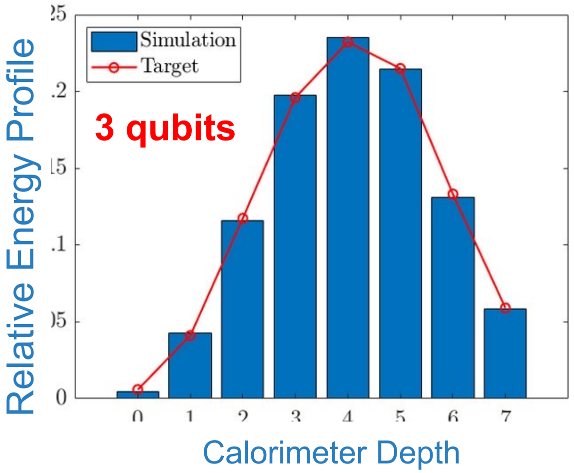
CERN openlab
S.Y. Chang

IBM qGAN can load probability distributions in quantum states

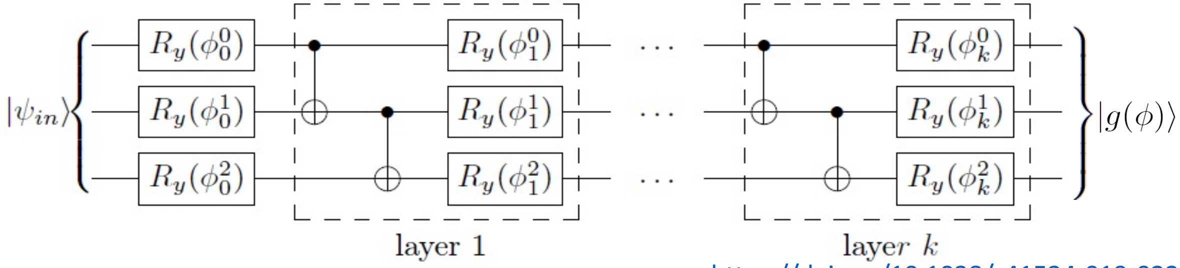
Simplify simulation problem

1D & 2D energy profiles from detector

Train a **hybrid classical-quantum** GAN to generate **average image**

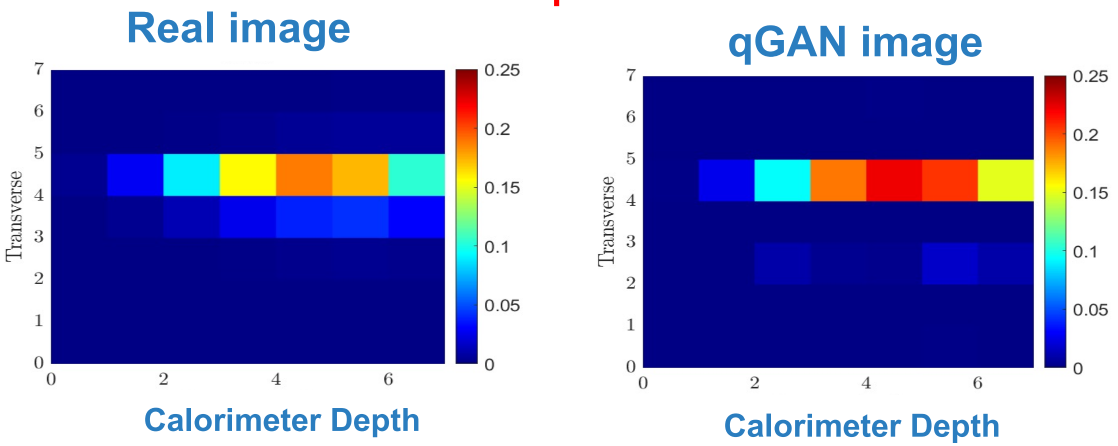


Quantum Generator: 3 R_y layers



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

6 qubits

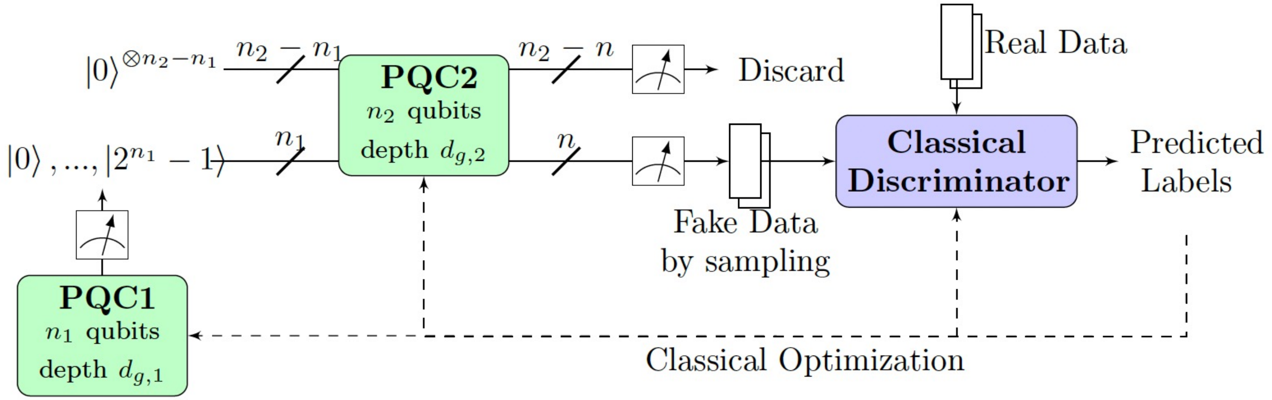


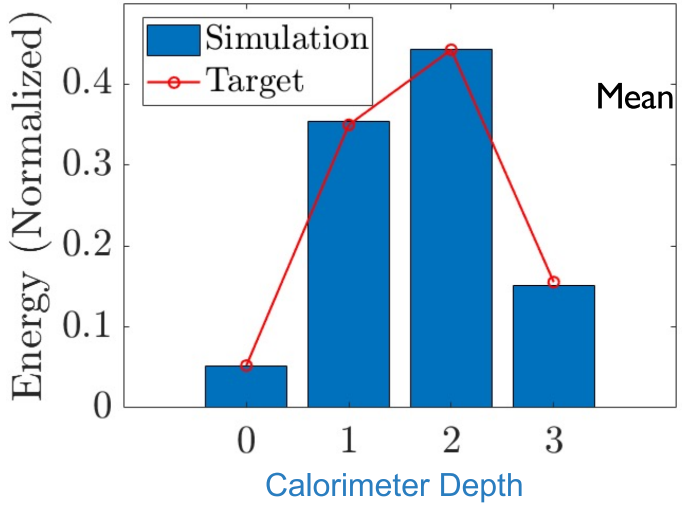
Need a way to **sample single images**

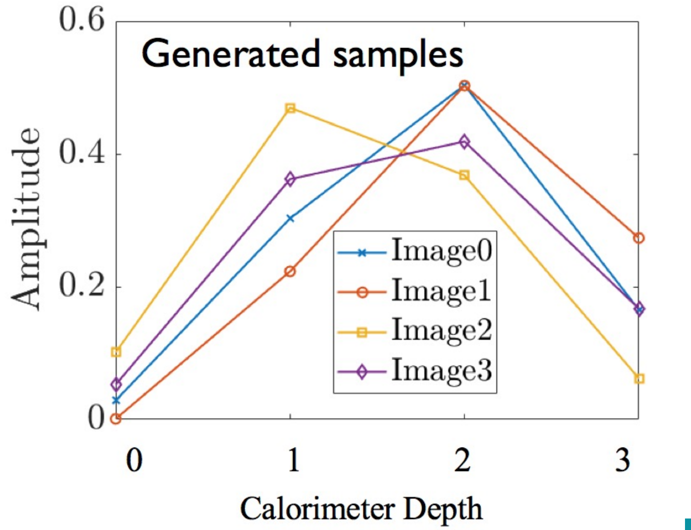
Extending the qGAN model

Two-steps quantum generator to sample images

- **PQC1 –** Reproduce distribution over images
- **PQC2 –** Reproduce amplitudes over pixels on one image







Benchmarks on hardware

Train models using noisy simulator and test the inference of the model on the superconducting (**IBMQ**) and trapped-ion (**IONQ**) quantum hardware

- For IBMQ machines, choose the qubits with the lowest CNOT gate error

Device	Readout error CX error	$D_{KL}/D_{KL,ind}$ $(\times 10^{-2})$
ibmq_jakarta	0.028 $1.367 \cdot 10^{-2}$	0.14 ± 0.14 6.49 ± 0.54
ibm_lagos	0.01 $5.582 \cdot 10^{-3}$	0.26 ± 0.11 6.92 ± 0.71
ibmq_casablanca	0.026 $4.58 \cdot 10^{-2}$	4.03 ± 1.08 6.58 ± 0.81
IONQ	NULL $1.59 \cdot 10^{-2}$	1.24 ± 0.74 10.1 ± 5.6

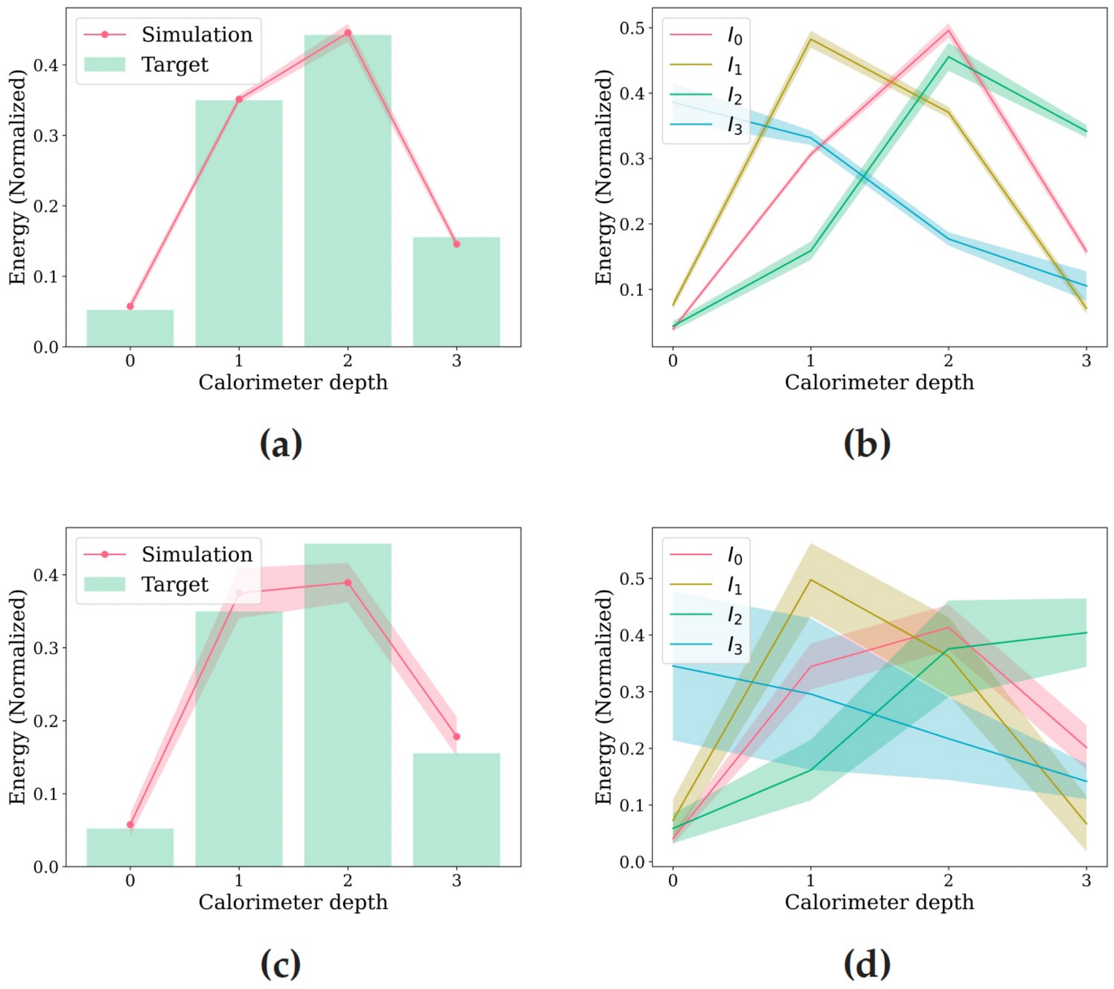
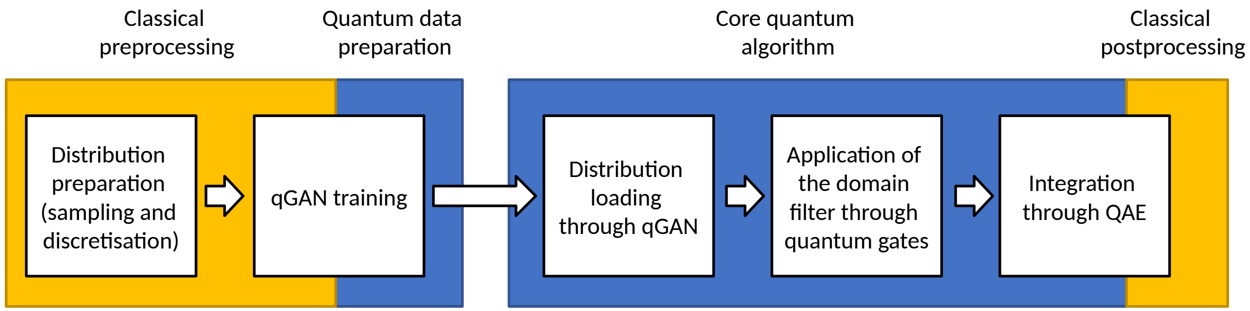
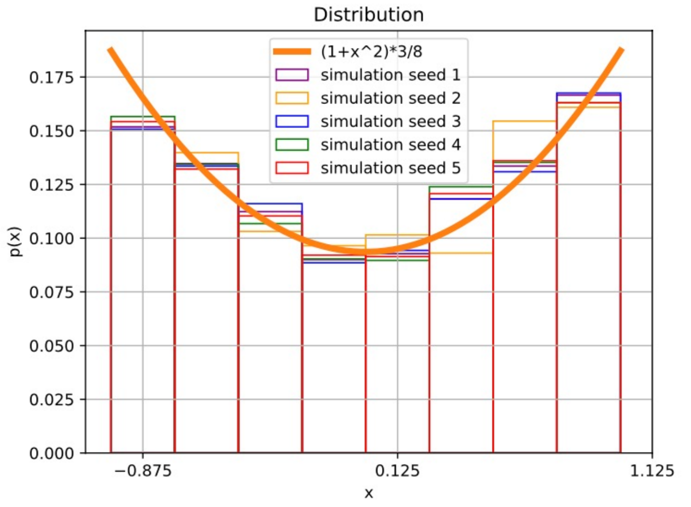


Figure 4: Mean (a,c) and individual images (b,d) obtained by inference test on ibmq_jakarta (a,b) and IONQ (c,d).

Quantum integration of elementary particle processes

Use **Quantum Amplitude Estimation** to accelerate Monte Carlo Integration
Data encoding into quantum states affects the quality of the integration
Test different approaches including **QGAN**





Loading of $1 + x^2$ distribution:

- 10k events
- 3 qubits
- best entanglement is the circular

M. Grossi, arxiv:2201.01547

FR-PHENO-2022-01

arXiv:2201.01547v1 [hep-ph] 5 Jan 2022

Quantum integration of elementary particle processes

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Abstract

We apply quantum integration to elementary particle-physics processes. In particular, we look at scattering processes such as $e^+e^- \to q\bar{q}$ and $e^+e^- \to q\bar{q}'W$. The corresponding probability distributions can be first appropriately loaded on a quantum computer using either quantum Generative Adversarial Networks or an exact method. The distributions are then integrated using the method of Quantum Amplitude Estimation which shows a quadratic speed-up with respect to classical techniques. In simulations of noiseless quantum computers, we obtain per-cent accurate results for one- and two-dimensional integration with up to six qubits. This work paves the way towards taking advantage of quantum algorithms for the integration of high-energy processes.

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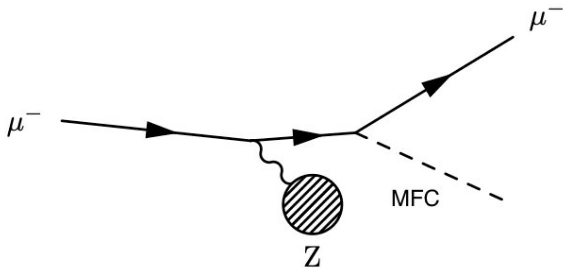
Quantum Circuit Born Machine for event generation

Muon Force Carriers predicted by several theoretical models:

- Could be detected by muon fixed-target experiments (FASER) or muon interactions in calorimeters (ATLAS).

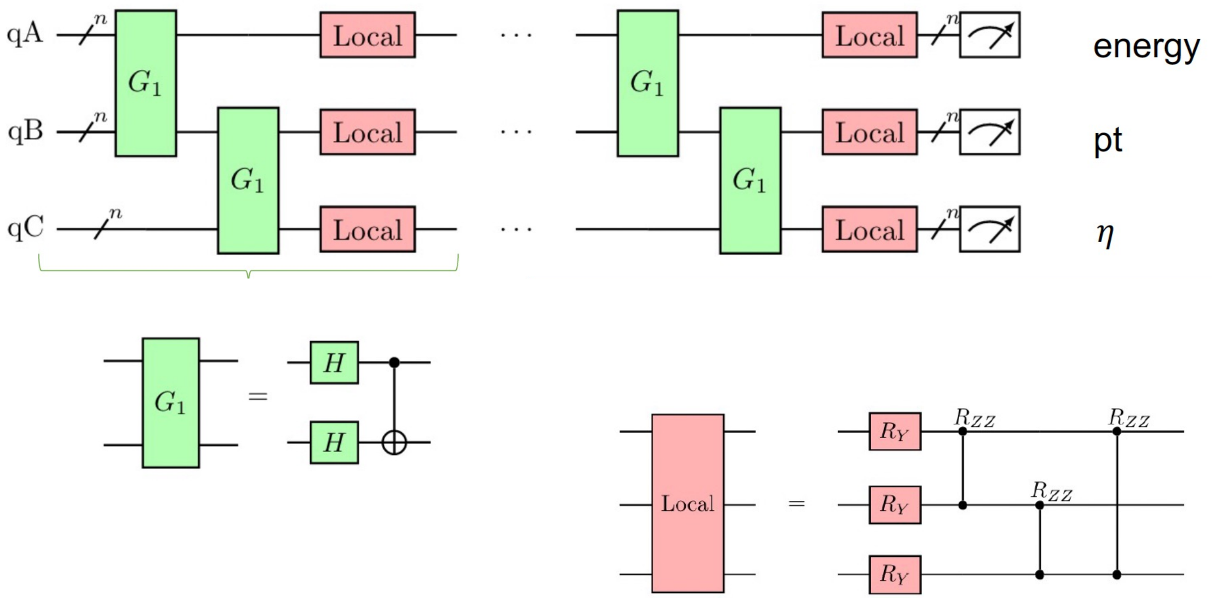


Generate **E, p_t, η** of outgoing muon and MFC

Sample from variational wavefunction $|\psi(\theta)\rangle$ with $p_\theta(x) = |\langle x|\psi(\theta)\rangle|^2$ given by the Born rule

Generate **discrete PDFs** (continuous in the limit #qubits → ∞)

Maximum Mean Discrepancy loss function and gaussian kernel with $\sigma \in [0.1,1,10,100]$



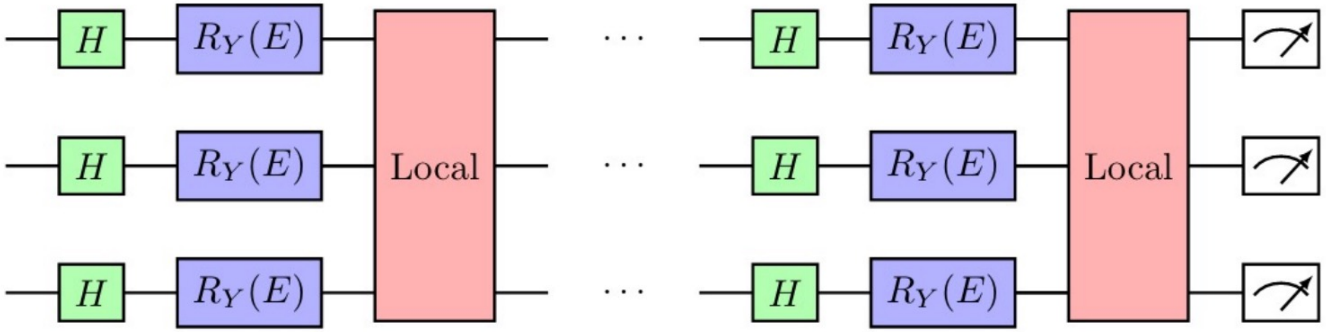
$$MMD(P,Q) = \mathbb{E}_{\substack{X\sim P\\Y\sim P}}[K(X,Y)] + \mathbb{E}_{\substack{X\sim Q\\Y\sim Q}}[K(X,Y)] - 2\mathbb{E}_{\substack{X\sim P\\Y\sim Q}}[K(X,Y)]$$

Galon, I, Kajamovitz, E et al. "Searching for muonic forces with the ATLAS detector". In: Phys. Rev. D 101, 011701 (2020)
Coyle, B., Mills, D. et al, "The Born supremacy". In: npj Quantum Inf 6, 60 (2020)

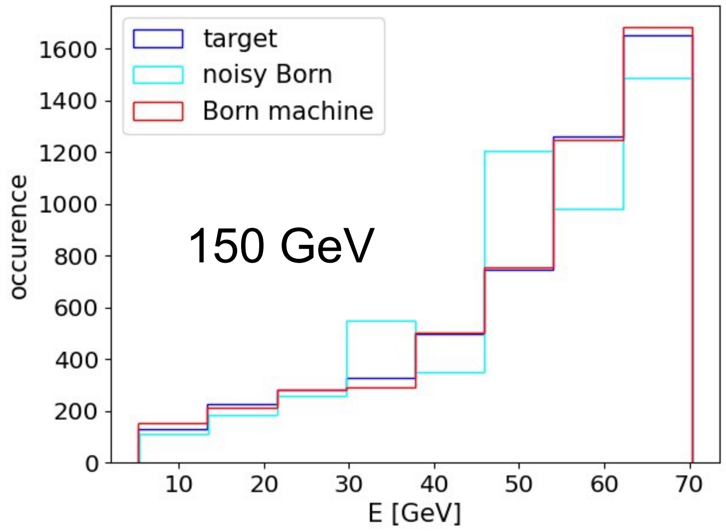
Conditional Born Machine

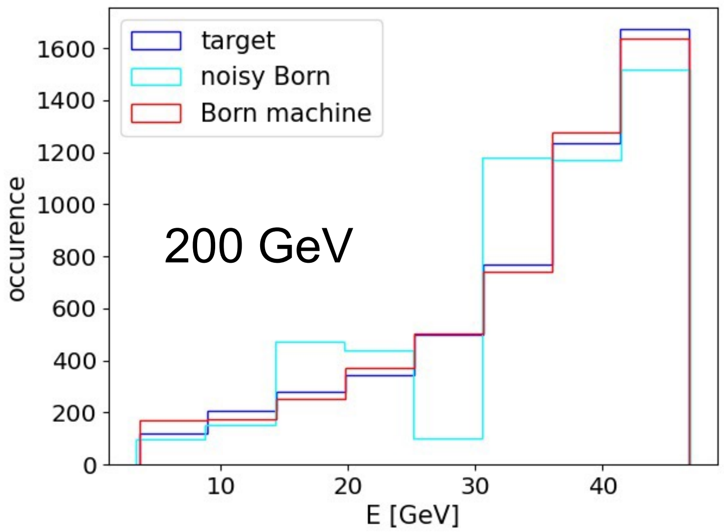
Encode $E_{\mu,i}$ condition using parametrized rotations

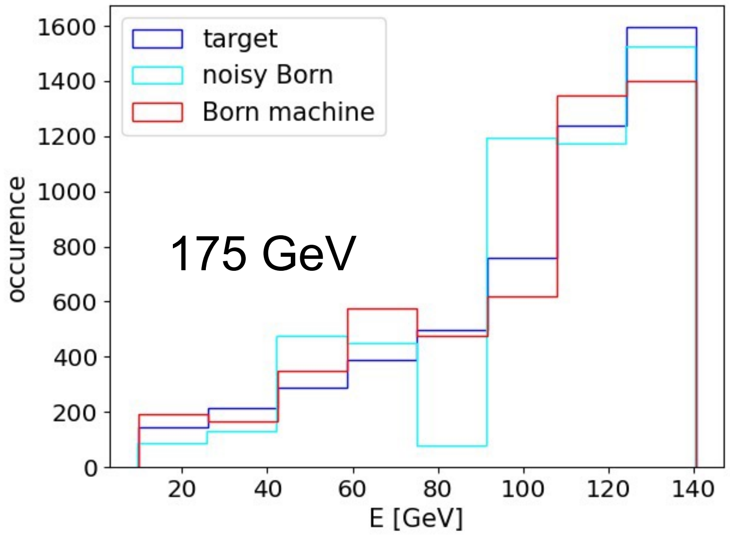
Interpolation: train on 150 and 200 GeV muons and predict 175 GeV signal



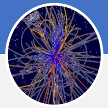
Data re-uploading makes the quantum circuit more expressive as function of the data
Noise model according to IBM Q Casablanca







Scientific Objectives



- Assess the **areas of potential quantum advantage** in HEP applications (QML, classification, anomaly detection, tracking)
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

Computing & Algorithms

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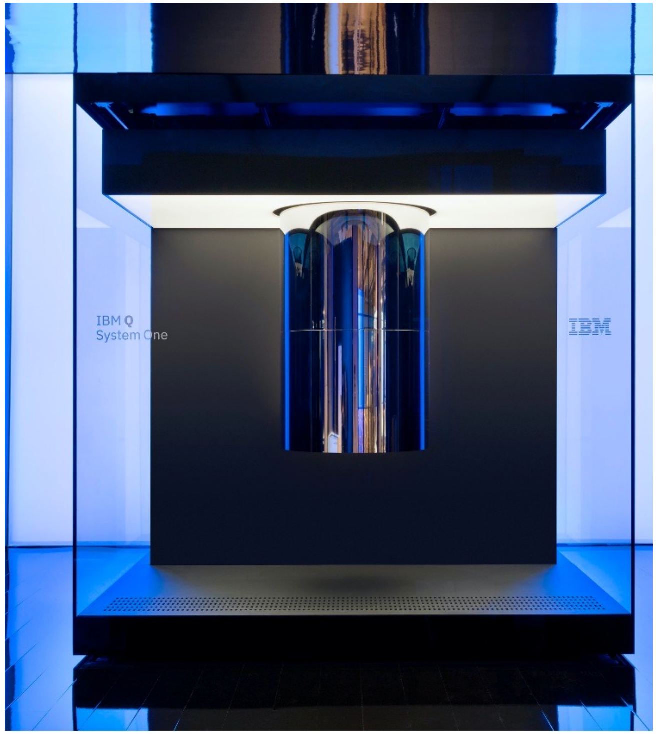
Hardware and Software Resources



- Focus on **tools for software development** and testing
- Access to **resources:** classical (simulators) and quantum hardware
  - Cluster with different quantum computing simulators for development up to 20-25 qubits
  - ATOS QLM appliance for simulations up to 34 qubits
  - Access to the IBM Q systems
- Evaluate **different hardware solutions**: digital (semiconductors, ions, photons) and annealer

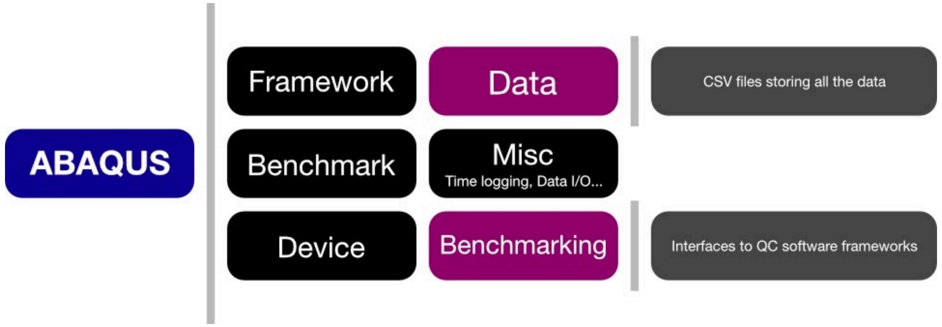
- Building shared experience on different **computing simulators**, real **NISQ hardware**, and hybrid infrastructures where **cloud computing**, **HPC resources** and **quantum computers** interact is key to capacity building for the future

ABAQUS - Automated Benchmarking of Algorithms for QUantum Systems

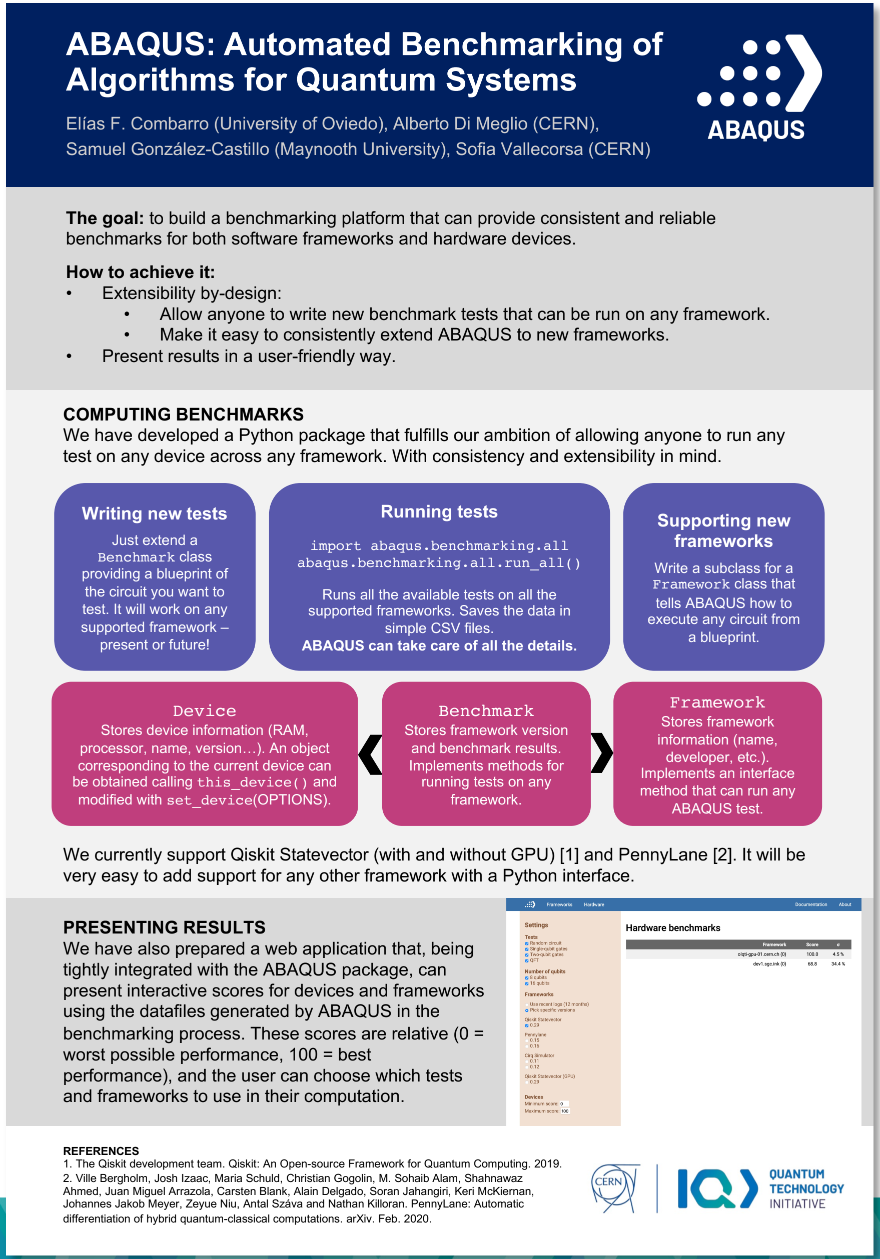
Benchmarking platform to benchmark for software frameworks and hardware devices.

- **Extensibility** by-design
- Present results in a **user-friendly** way.
- A **web application** to interactively present results

Currently supports Qiskit State Vector (with and without GPU), Cirq and PennyLane



Gonzalez Castillo S. *et al.*, EQTC2021



ABAQUS: Automated Benchmarking of Algorithms for Quantum Systems

Elías F. Combarro (University of Oviedo), Alberto Di Meglio (CERN), Samuel González-Castillo (Maynooth University), Sofia Vallecorsa (CERN)

The goal: to build a benchmarking platform that can provide consistent and reliable benchmarks for both software frameworks and hardware devices.

How to achieve it:

- Extensibility by-design:
  - Allow anyone to write new benchmark tests that can be run on any framework.
  - Make it easy to consistently extend ABAQUS to new frameworks.
- Present results in a user-friendly way.

COMPUTING BENCHMARKS

We have developed a Python package that fulfills our ambition of allowing anyone to run any test on any device across any framework. With consistency and extensibility in mind.

Writing new tests

Just extend a `Benchmark` class providing a blueprint of the circuit you want to test. It will work on any supported framework – present or future!

Running tests

```
import abaqus.benchmarking.all
abaqus.benchmarking.all.run_all()
```

Runs all the available tests on all the supported frameworks. Saves the data in simple CSV files.
ABAQUS can take care of all the details.

Supporting new frameworks

Write a subclass for a `Framework` class that tells ABAQUS how to execute any circuit from a blueprint.

`Device`

Stores device information (RAM, processor, name, version…). An object corresponding to the current device can be obtained calling `this_device()` and modified with `set_device`(OPTIONS).

`Benchmark`

Stores framework version and benchmark results. Implements methods for running tests on any framework.

`Framework`

Stores framework information (name, developer, etc.). Implements an interface method that can run any ABAQUS test.

We currently support Qiskit Statevector (with and without GPU) [1] and PennyLane [2]. It will be very easy to add support for any other framework with a Python interface.

PRESENTING RESULTS

We have also prepared a web application that, being tightly integrated with the ABAQUS package, can present interactive scores for devices and frameworks using the datafiles generated by ABAQUS in the benchmarking process. These scores are relative (0 = worst possible performance, 100 = best performance), and the user can choose which tests and frameworks to use in their computation.

REFERENCES

1. The Qiskit development team. Qiskit: An Open-source Framework for Quantum Computing. 2019.
2. Ville Bergholm, Josh Izaac, Maria Schuld, Christian Gogolin, M. Sohaib Alam, Shahnawaz Ahmed, Juan Miguel Arrazola, Carsten Blank, Alain Delgado, Soran Jahangiri, Keri McKiernan, Johannes Jakob Meyer, Zeyue Niu, Antal Száva and Nathan Killoran. PennyLane: Automatic differentiation of hybrid quantum-classical computations. arXiv. Feb. 2020.

Research Collaborations (various stages of maturity)

Organizations and Projects

QUANTUM FLAGSHIP

QuantHEP

esa

Industry

Google

IBM

IBM Q-Net

intel

Amazon Braket

aws

Microsoft

Xanadu

Atos

PASQAL

Cambridge Quantum Computing

QILIMANJARO QUANTUM · TECH

DESY.

TUM

lrz

ETH zürich

EPFL

UNIVERSITÉ DE GENÈVE

UK NATIONAL QUANTUM TECHNOLOGIES PROGRAMME

cea

cnrs IN2P3

INFN Istituto Nazionale di Fisica Nucleare

Universitas Studii Paduani

Universitas Studiorum Insubriae

Università degli Studi di Milano Bicocca

iit Istituto Italiano di Tecnologia

QuTech

BSC

Universidad de Oviedo

Fermilab

Oak Ridge National Laboratory

instituto de telecomunicações

Politechnika Warszawska – Warsaw University of Technology

Helsingin Yliopisto

Academia, Research Labs and Agencies

Orta Doğu Teknik Üniversitesi – Middle East Technical University Northern Cyprus Campus

University of Waterloo

ICEPP The University of Tokyo

STUDY ON IMPACTS OF QUANTUM NOISES ON QGAN TRAINING

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[1]CERN, Openlab, [2]EPFL, [3] RWTH Aachen University [4] The Cyprus Institute, [5] Deutsches Elektronen-Synchrotron DESY, [6]MIT, [7]University of Bath

INTRODUCTION

- **Artificial noises** are often injected in machine learning for a more robust, more stable and faster converging model.
- Current and near future quantum devices still have **considerable levels of noise**.
- Possibility to replace the artificial noise in classical ML with the intrinsic noise in quantum ML (QML).

OBJECTIVES

- Investigate the **impact of different errors** in the training of quantum Generative Adversarial Networks (qGAN) [1] for a simplified High-Energy Physics (HEP) use case.
- Provide a broad exploratory study to unfold the hidden impact of noise in QML.

ACAT2021 (arxiv:2203.01007)
Collaboration with DESY, RWTH AACHEN UNIVERSITY
(see K. Borras' talk on wednesday)

getting state $|k\rangle$ = normalized energy at pixel k.

- Input dataset = scalars following the real energy distribution

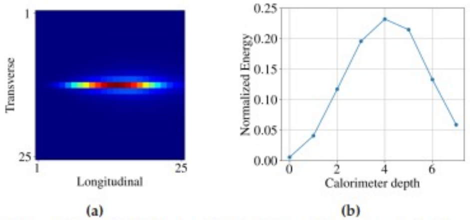


Figure 2: (a) Original calorimeter output generated by *Geant4*. (b) Reduced energy distribution used for our qGAN training.

REFERENCES

[1] Christa Zoufal, Aurélien Lucchi, and Stefan Woerner. Quantum generative adversarial networks for learning and loading random distributions. *npj Quantum Information*, 5(1):103, Nov 2019.

QUANTUM GAN

- **Hybrid model** with a n-qubit quantum generator and a classical discriminator [1]

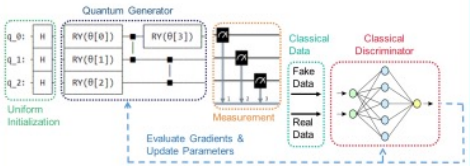


Figure 3: Schematic Diagram of qGAN.

- Relative entropy (or *Kullback-Leibler (KL) divergence*) $D_{KL}(p\|q) = \sum_j p(j) \log \frac{p(j)}{q(j)}$ as accuracy metrics.

...ERPARAMETER SCAN

...perform a scan on different **subsets of hyperpa...eters**: decay rate γ, generator lr_g, and discrimi...r learning rate lr_d.

... the qGAN training using a noise model **with ...dout error** in form of bit flips occurring indepen...tly for each qubit with a flip probability p.

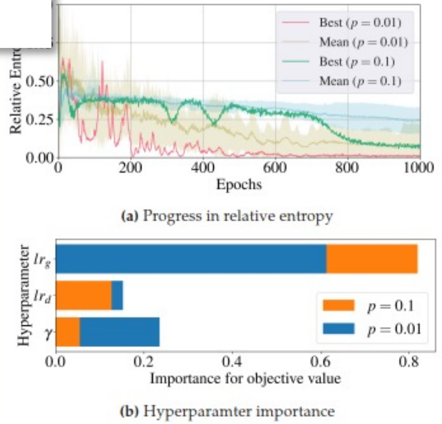


Figure 5: Results of the scan on different hyperparameters for the readout error $p = 0.01$ and 0.1

- Higher relative entropy for higher noise level, even with the optimal hyperparameters.
- Impact of generator learning rate becomes higher as the flip probability increases.

INSTABILITY OF QGAN TRAINING

- Repeat the qGAN training with the *qiskit* noise model with readout error only using the same hyperparameters and **investigate its statistical error**.

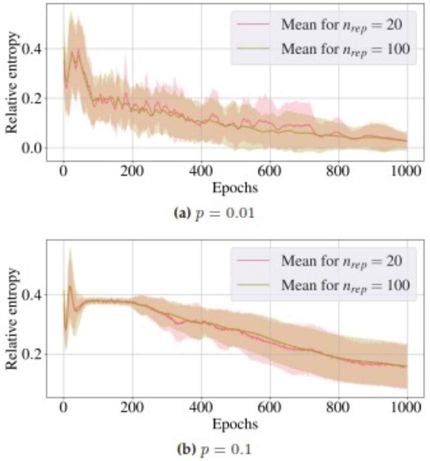


Figure 4: Progress in relative entropy averaged over n_{rep} = 20 and 100 runs for $p = 0.01$ and 0.1.

Flip probability p	$n_{rep} = 20$	$n_{rep} = 100$
0.01	0.026 ± 0.028	0.028 ± 0.040
0.05	0.029 ± 0.022	0.027 ± 0.020
0.1	0.153 ± 0.097	0.159 ± 0.077

Table 1: Relative entropy at the end of the training

- The model is stable on the "ensemble" of simulations, but unstable for the individual runs.
  → Fixed standard deviation despite increase in the number of simulations.

DISCUSSION

- **The instability of the qGAN model** cannot be resolved even with large number of simulations.
  → Further study going on to find the origin of the instability.
- Small levels of quantum noise help to improve the performance of the model, while error mitigation is required for large noise.
- Effect of error mitigation in the full noise model and the real quantum hardware needs to be further studied.

ERROR MITIGATION

- We compare the training results with and without **error mitigation method** implemented by *qiskit*.

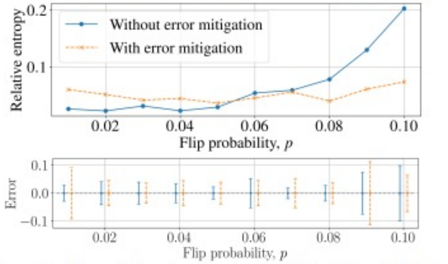


Figure 6: Mean (above) and standard deviation (below) of the final relative entropy, averaged over 20 simulations, with and without error mitigation w.r.t. the readout error.

- Low readout error ($p < 0.06$) helps the qGAN training, while error mitigation plays an important role for high readout error.
- Large standard deviation in the relative entropy which cannot be overcome with error mitigation.

INCLUDING CNOT ERROR

- We run the training with a custom noise model consisting of 2.5% readout noise per qubit and 1.5% two qubit gate level noise (called CNOT error).
- We found new optimized hyperparameters to reduce the number of epochs to only 300 while reaching a good accuracy.

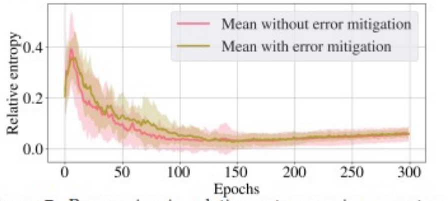


Figure 7: Progression in relative entropy using a custom noise model with and without error mitigation.

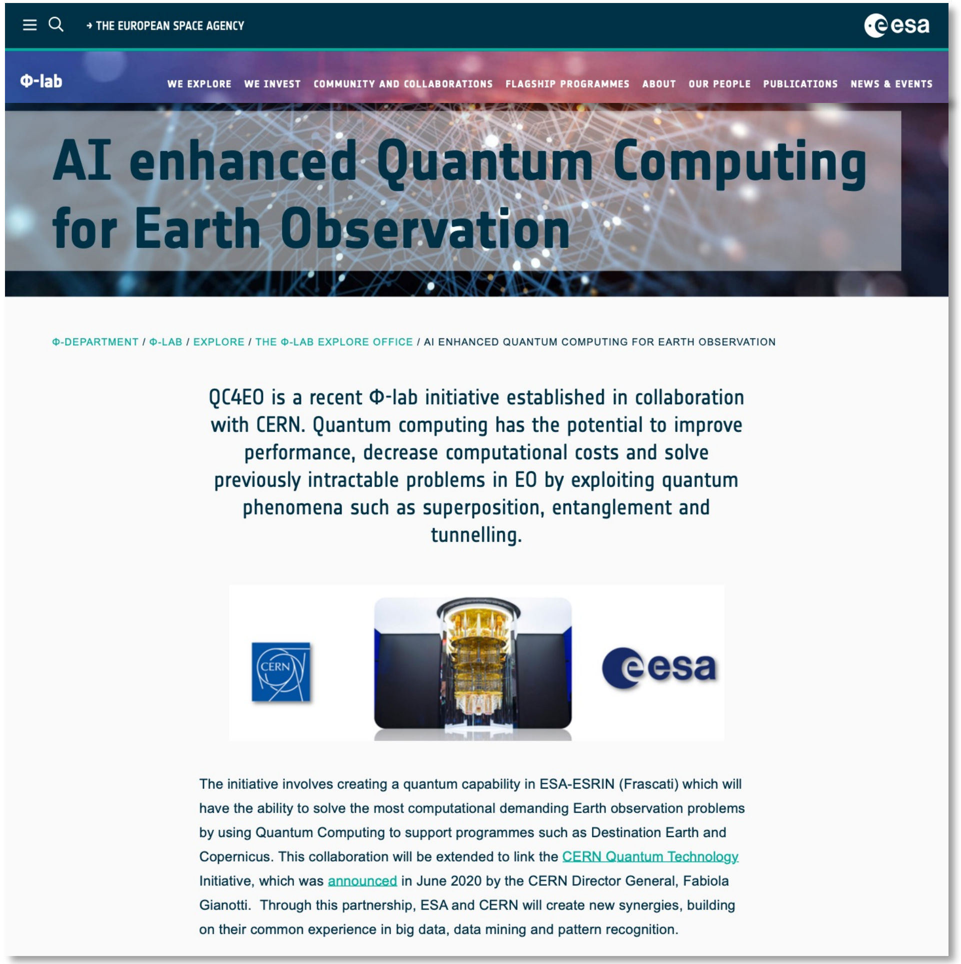
- For the chosen noise levels one cannot see any improvement when including error mitigation.

ONGOING RESEARCH

- Train the qGAN on real quantum hardware.
- Apply other error mitigation methods and compare the resulting outcomes.

Synergies with other sciences

The ESA-CERN Joint Announcement at Phi-Week 2020



→ THE EUROPEAN SPACE AGENCY

Φ-lab

WE EXPLORE WE INVEST COMMUNITY AND COLLABORATIONS FLAGSHIP PROGRAMMES ABOUT OUR PEOPLE PUBLICATIONS NEWS & EVENTS

AI enhanced Quantum Computing for Earth Observation

Φ-DEPARTMENT / Φ-LAB / EXPLORE / THE Φ-LAB EXPLORE OFFICE / AI ENHANCED QUANTUM COMPUTING FOR EARTH OBSERVATION

QC4EO is a recent Φ-lab initiative established in collaboration with CERN. Quantum computing has the potential to improve performance, decrease computational costs and solve previously intractable problems in EO by exploiting quantum phenomena such as superposition, entanglement and tunnelling.

The initiative involves creating a quantum capability in ESA-ESRIN (Frascati) which will have the ability to solve the most computational demanding Earth observation problems by using Quantum Computing to support programmes such as Destination Earth and Copernicus. This collaboration will be extended to link the CERN Quantum Technology Initiative, which was announced in June 2020 by the CERN Director General, Fabiola Gianotti. Through this partnership, ESA and CERN will create new synergies, building on their common experience in big data, data mining and pattern recognition.

Quantum Convolutions

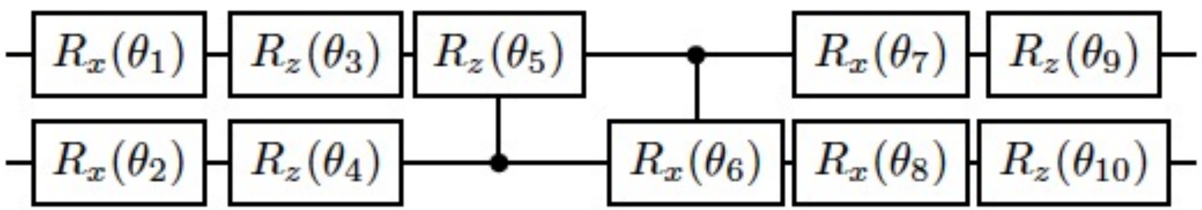
Chang, Su Yeon et al., QTNML2021@NeurIPS2021

Convolutional Filters[1] as Parameterized Quantum Circuits (PQC) with single-qubit and two-qubit operations.

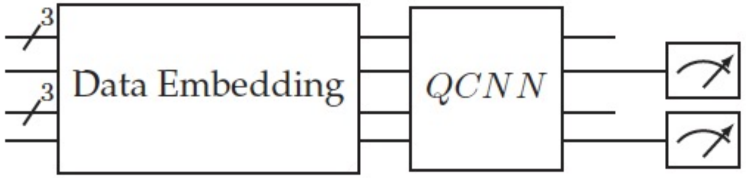
- Reduce risk of barren plateau

Alternative architecture: different parameters in each convolutional filters

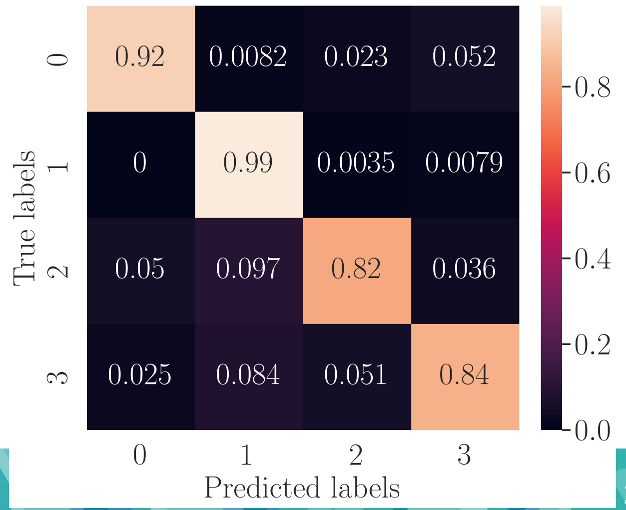
- Increased model complexity and flexibility



N-class classification by measuring the probability distribution for $\log_2 N$ qubit and using categorical cross entropy.



Confusion matrix of 4-class MNIST classification



[1] T. Hur, L. Kim, and D. K. Park. Quantum convolutional neural network for classical data classification, 2021.

Summary

The QTI coordinates **quantum research at CERN**

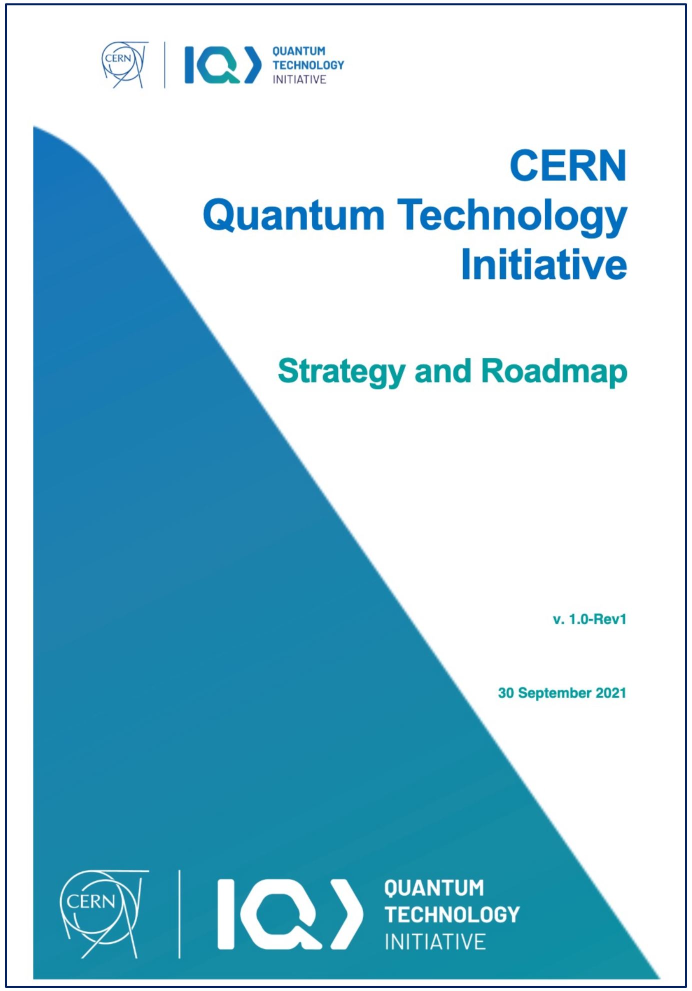
- Quantum Computing is a wide active area

Extensively investigating **QC and QML applications to HEP**

- Initial set of prototypes for different applications
- **Move on to more robustness studies**

Setting in place **access to resources (classical and quantum)** to ease community R&D

Build **synergies and joint projects** beyond HEP



https://zenodo.org/record/5553775

Thanks!

Sofia.Vallecorsa@cern.ch

CERN

IQ

QUANTUM
TECHNOLOGY
INITIATIVE

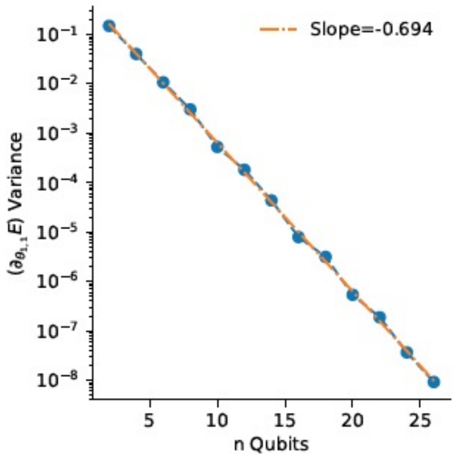
Model Convergence and Barren Plateau

Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)

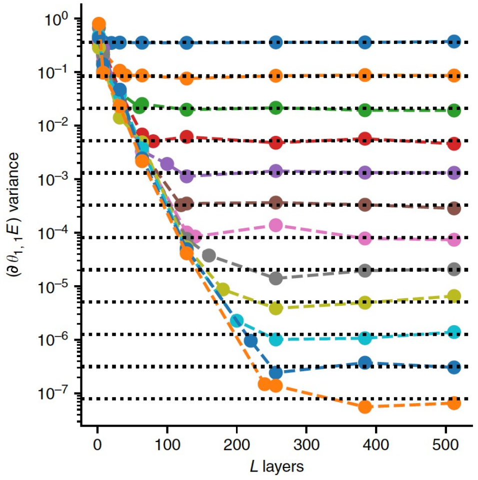
- Convergence still possible if gradients consistent between batches.

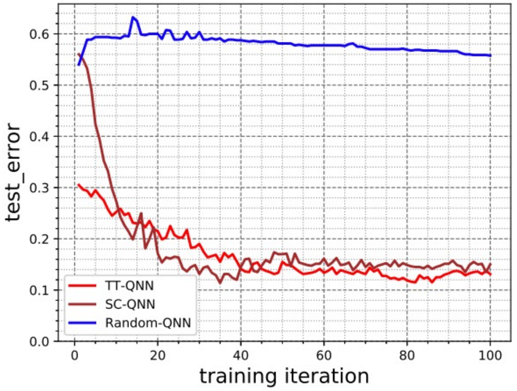
Quantum gradient decay exponentially in the number of qubits

- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.,* arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12, 6961 (2021))

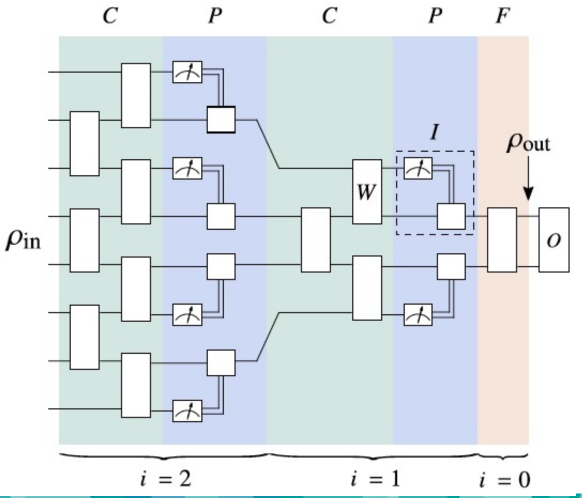


J. McClean *et al.*, arXiv:1803.11173





TTN for MNIST classification (8 qubits), Zhang *et al.,* arXiv:2011.06258

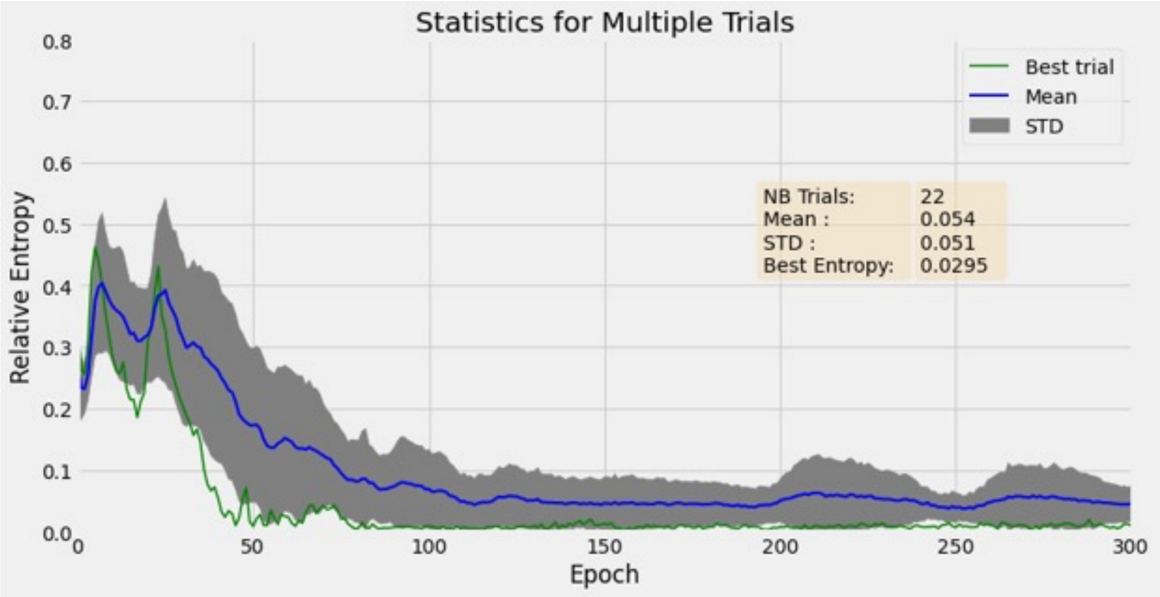


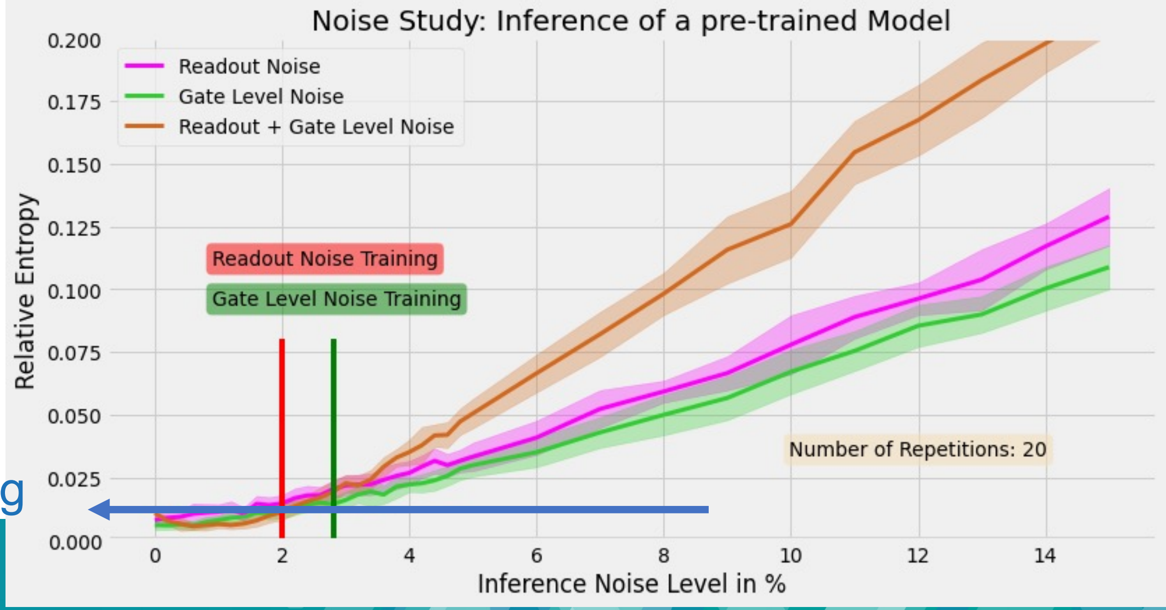
QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011

F. Rehm, Grid2021 conference
https://indico.jinr.ru/event/1086/contributions/13067/

Noise studies for qGAN

- **Gate + readout noise (IBM Belem) seem to improve convergence**
  - Noiseless simulation converges at ~300 epochs
- **Stable performance of the inference process up to 2% error probability**





Rel Entropy measured during training

QML implementations

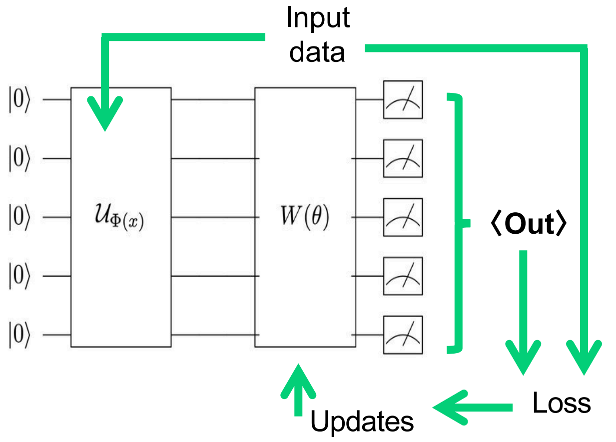
Variational algorithms

Parametric ansatz

Can use **gradient-free** methods

or **stochastic gradient-descent**

Data Embedding can be **learned**



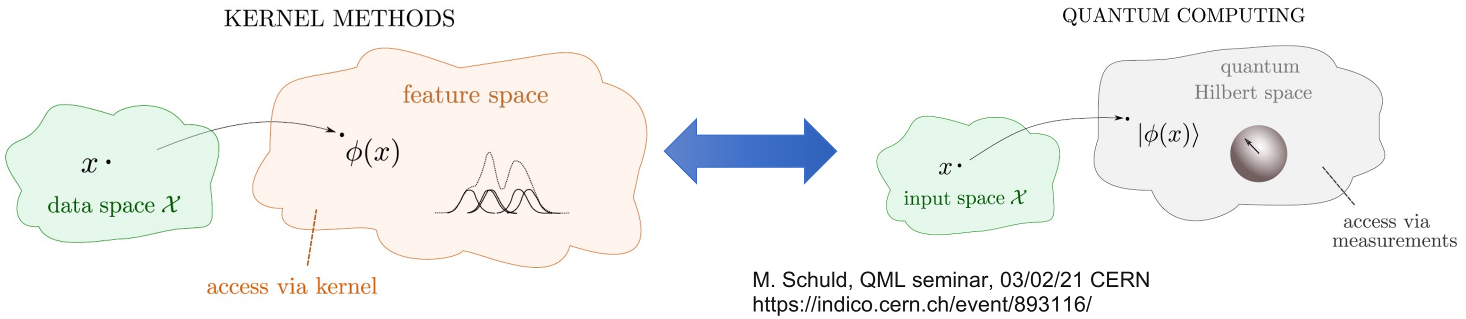
Kernel methods

Feature maps as **quantum kernels**

Use classical **kernel-based training**

Convex losses, **global** minimum

Compute pair-wise distances in N_{data}



M. Schuld, QML seminar, 03/02/21 CERN
https://indico.cern.ch/event/893116/

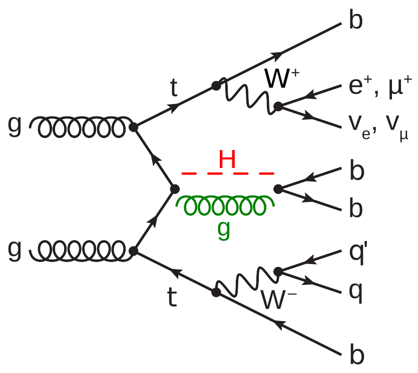
Near term **quantum hardware** access & integration with classical computing?

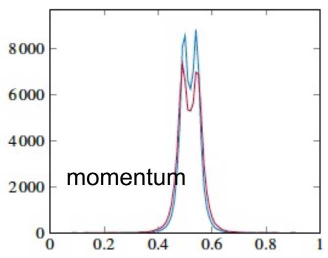
V. Belis, S. Gonzalez-Castillo
BQiT 2021
vCHEP2021
arXiv:2104.07692

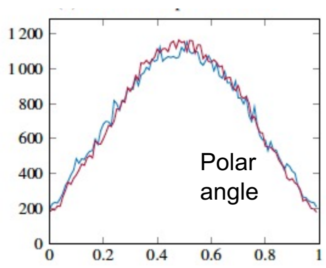
Quantum SVM for Higgs classification

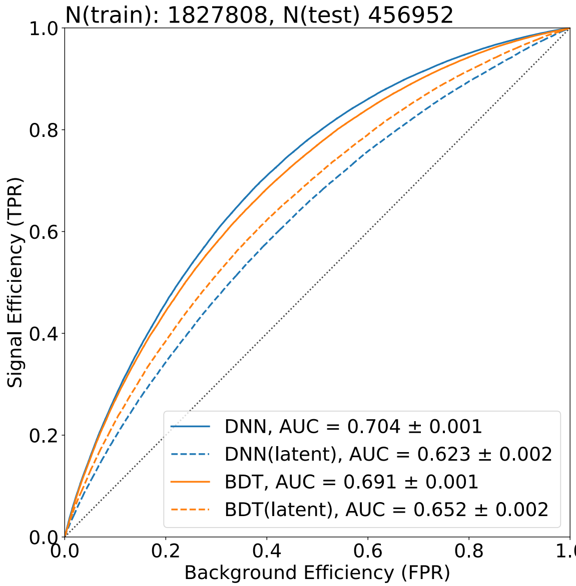
Classical models trained on 67 features

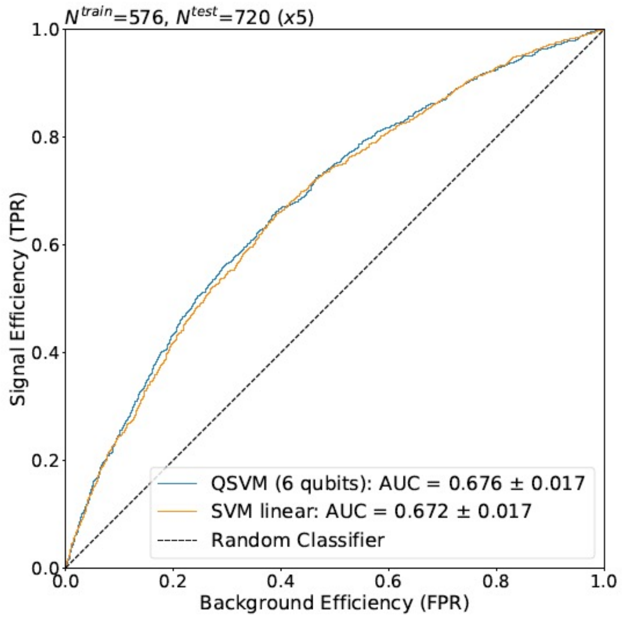
Test several dimensionality reduction strategies (PCA, AutoEncoder, Kmeans..)



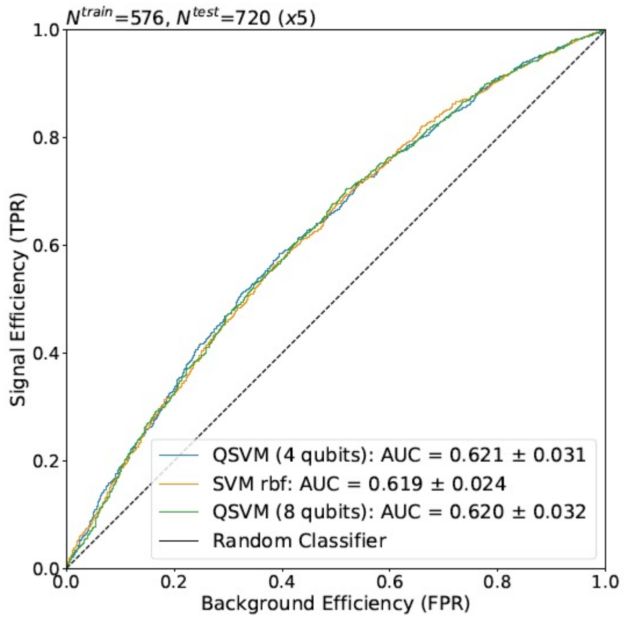








(b) Models trained on the original input features (67), discarding the 3 least informative ones (64).

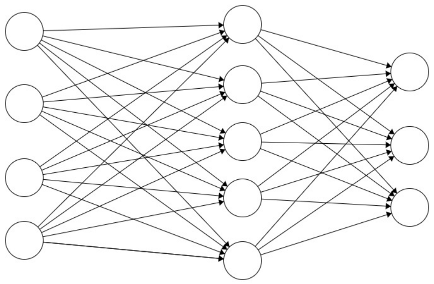


(a) Models trained on the AE latent space features (16).

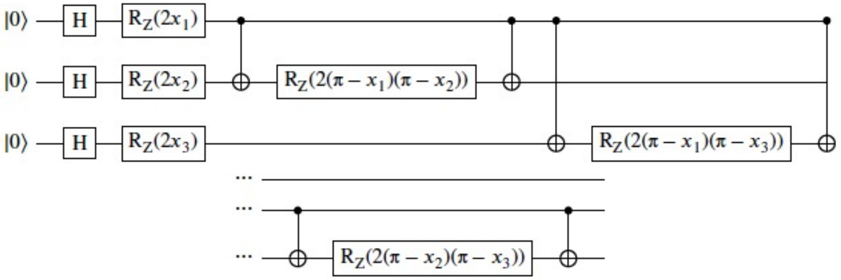
VQC for Higgs classification

Classical dense neural network to reduce dimensionality

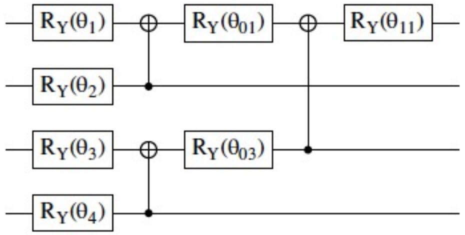
- 4 qubits, 8 variables



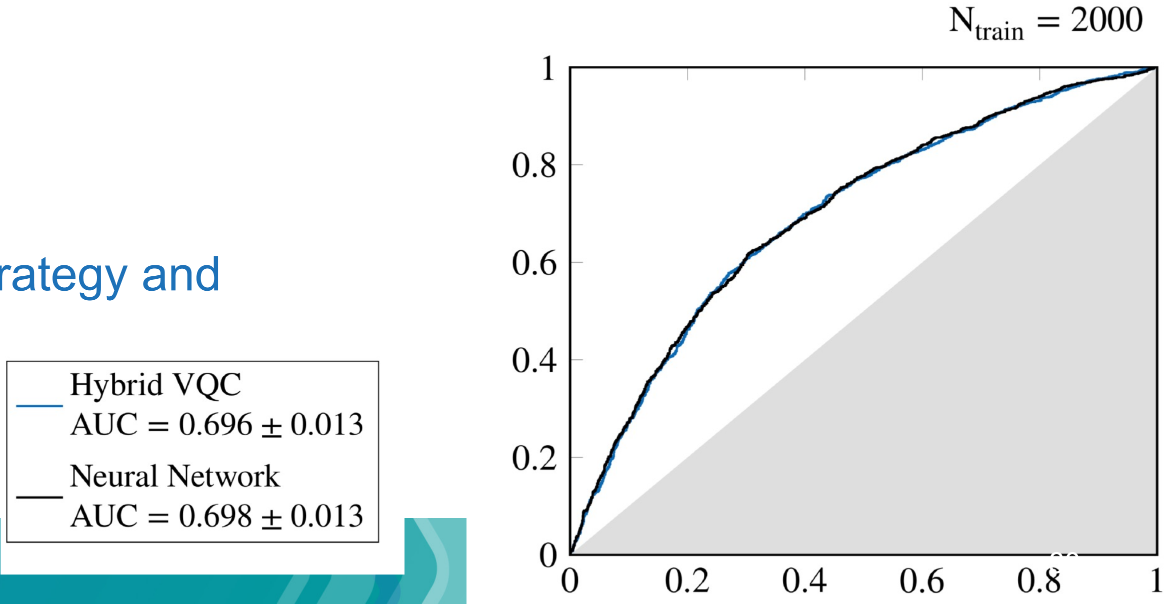
ZZ feature map with data-re-uploading



2-local variational form

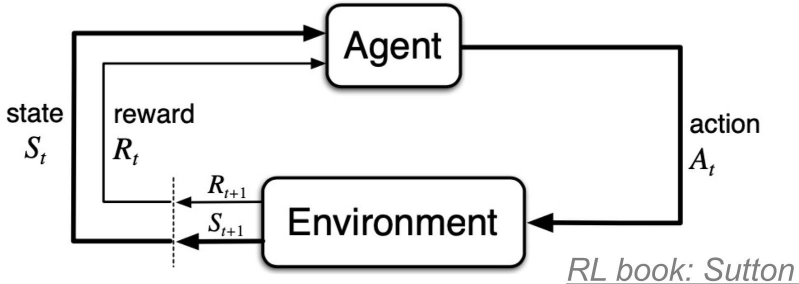


Simultaneous training of classical feature extraction strategy and quantum classifier improves the accuracy



M. Shenk, V. Kain
BQiT 2021
2021 CERN openlab Tech Workshop

Reinforcement learning in a nutshell



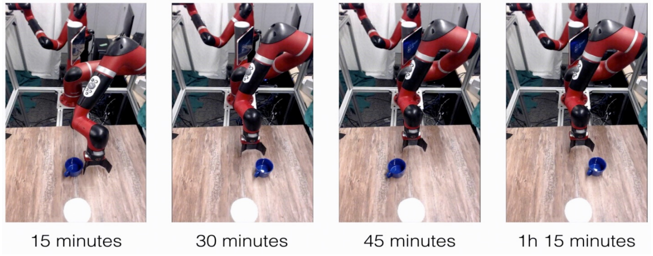
RL book: Sutton & Barto

Agent interacts with environment

- **Receives reward after every action**
- Learns through **trial-and-error**

Decision making

- Agent follows certain **policy** $\boldsymbol{\pi}$: $S \rightarrow A$
- **Goal: find optimal policy** $\boldsymbol{\pi}^*$
- **Optimal ⇔ maximizing return:** $G_t = \sum_k \gamma^k R_{t+k}$



source

Expected return can be estimated by ***value function Q(s, a)***

- **Best action chosen through a *greedy policy:*** *take action that maximizes Q(s,a)*
- **Not a priori known, but can be learned iteratively**
- *This work:* **Q-learning** – learn Q(s, a) using **function approximator**
  - DQN: Deep Q-learning *(feed-forward neural network)*
  - QBM-RL *(Quantum Boltzmann Machine)*

Q-learning

Free Energy RL: clamped QBM

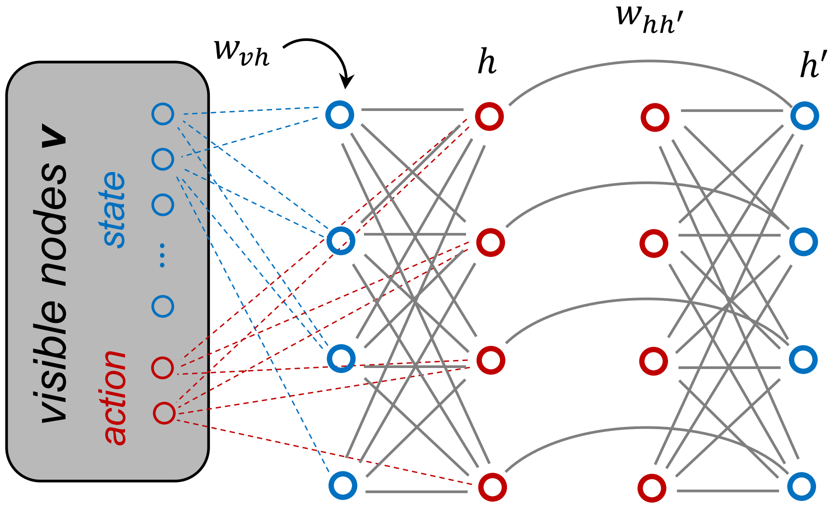
- **Network of coupled, stochastic, binary units** (spin up / down)
- $\hat{Q}(s,a)$ ≈ **negative free energy** of classical spin configurations c
- **Sampling** c using **(simulated) quantum annealing**
- **Clamped:** visible nodes not part of QBM; accounted for as biases
- **Using 16 qubits of D-Wave Chimera graph**
- **Discrete, binary-encoded** state and action spaces

DQN: Q-net

- **Feed-forward, dense** neural network
- 2 hidden layers, 8 nodes each (≈ Chimera graph)
- Can handle **discrete, binary-encoded** state and action spaces

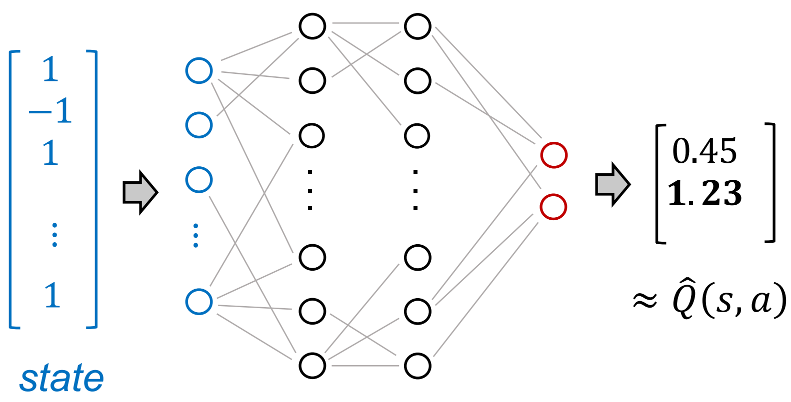
Learning: update Q by applying **temporal difference rule** to QBM and Q-net weights, respectively

Clamped QBM



$$\hat{Q}(s,a) \approx -F(\boldsymbol{v}) = -\langle H_{\boldsymbol{v}}^{\text{eff}} \rangle - \frac{1}{\beta}\sum_c \mathbb{P}(c|\boldsymbol{v}) \log \mathbb{P}(c|\boldsymbol{v})$$

Q-net



Beam steering through RL

- Fixed target experiments at CERN Super Proton Synchrotron
- OpenAI gym template
- **Action:** deflection angle (up or down by fixed amount)
- **State:** beam position at BPM
- **Reward:** integrated beam intensity on target
  - Additional reward for success