Quantum Computing at CERN

QUANTUM TECHNOLOGY INITIATIVE

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AI and Quantum Research - CERN openlab

CERN

CERN QTI and its Roadmap

CERN established the QTI in 2020

- Roadmap in 2021
- Publicly available on Zenodo
  - Accessed more than 5000 times

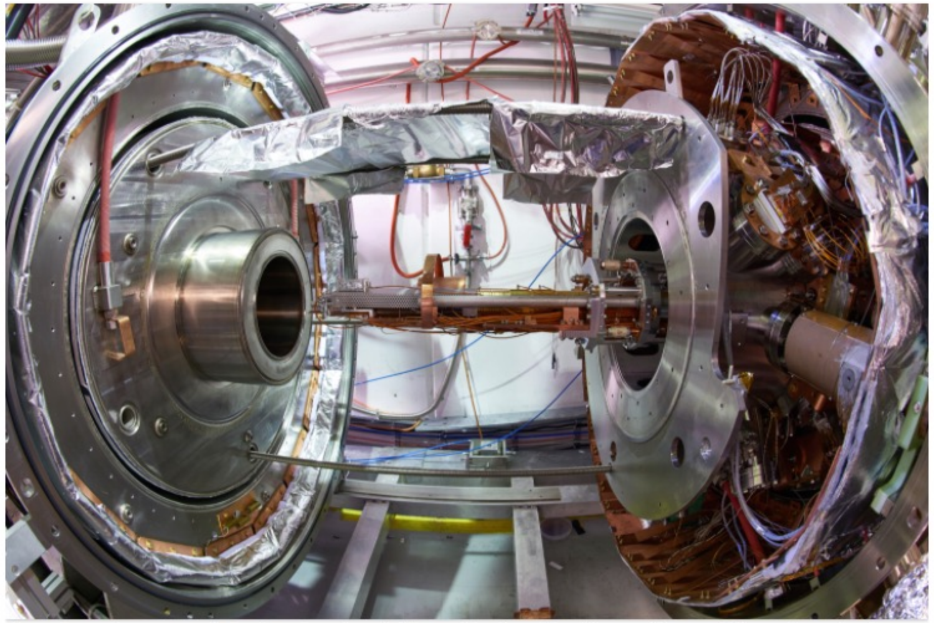
https://doi.org/10.5281/zenodo.5553774

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)

Computing and Algorithms

Sensing

Theory and Simulation

Communication

APPLICATIONS | NEWS

CERN unveils roadmap for quantum technology

4 November 2021

QUANTUM TECHNOLOGY INITIATIVE

Credit: CERN

Quantum Computing at CERN

- QC is one of the four research areas in the CERN QTI
- Understand which applications can profit from quantum algorithms
  - Choose **representative use cases**
  - Understand **challenges and limitations** (on NISQ and fault tolerant hardware)
  - **Optimize** quantum algorithms
- Quantum Machine Learning algorithms are a primary candidate for investigation
  - Increasing use of ML in many computing and data analysis flows
  - Can be built as **hybrid models** where quantum computers act as accelerators
  - Efficient data handling is a challenge

Quantum Machine Learning

Use **Quantum Computing** to accelerate **ML/DL.**

Quantum circuits are **differentiable** and can be trained **minimizing a cost function** dependent on training data:

1. **Feature extraction** and **data encoding**
   - How to represent classical data in quantum states?
2. **Model definition** (kernel based or variational)
   - Design wrt data
3. **Optimisation** and **convergence in Hilbert space**
   - Convergence vs expressivity
   - Barren plateau and vanishing gradients
   - Gradient-free or gradient-based optimisers
   - …

Different tools can enable hybrid computations

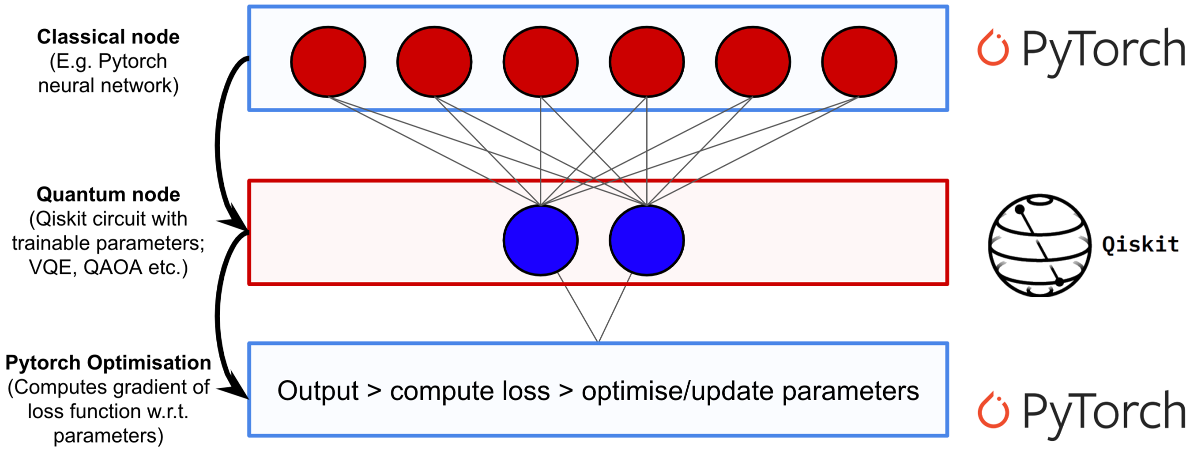


Image credit Qiskit.org/textbook

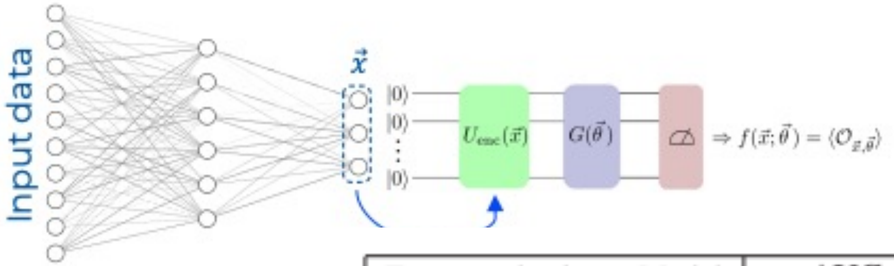
Dimensionality reduction and data embedding

Dimensionality reduction/feature extraction

- Reduce size of classical data
- Optimize input (PCA, Auto-Encoders..)
- **Pre-trained or co-trained** in hybrid setup

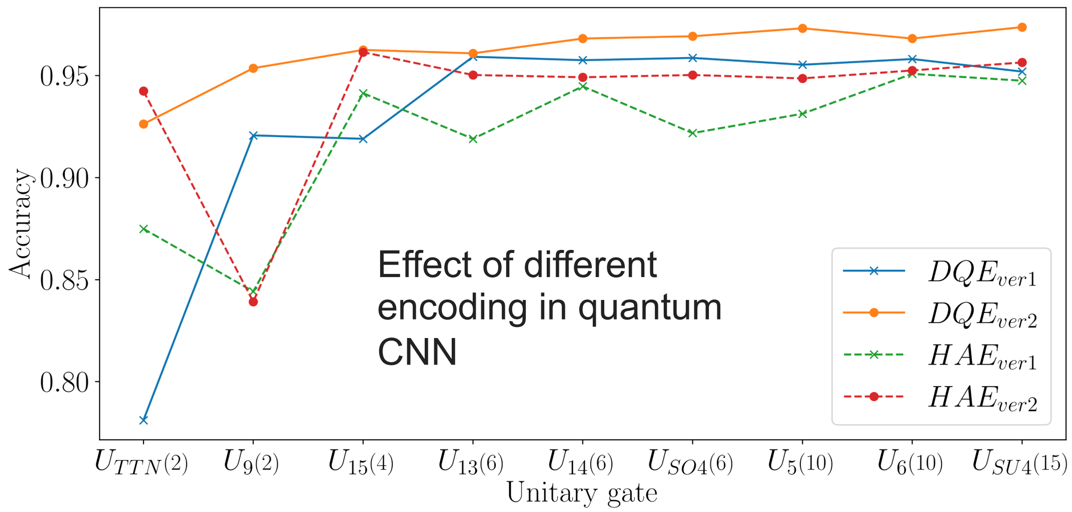
Data embedding : compromise between exponential compression and circuit depth

- **Amplitude Encoding** (exponential compression in n_{qubits})
- **Dense Qubit Encoding** (one-to-one)
- **Hybrid Angle Encoding** (bx2^m values in bxm qubits)



Belis, Vasilis, et al. "**Higgs analysis with quantum classifiers**." *EPJ Web of Conferences*. Vol. 251. EDP Sciences, 2021.

Feature selection + Model	AUC
AUC + QSVM	0.66 ± 0.01
PyTorch AE + QSVM	0.62 ± 0.03
AUC + SVM rbf	0.65 ± 0.01
PyTorch AE + SVM rbf	0.62 ± 0.02
KMeans + SVM rbf	0.61 ± 0.02



S.Y. Chang, poster at "**Quantum Tensor Network in Machine Learning**, NeurIPS 2021

Model definition

Variational algorithms

Parametric ansatz

Gradient-free or **gradient-based** optimization

Data Embedding can be **learned**

Can design architectures to leverage data symmetries[1]

1 Bogatskiy, Alexander, et al. "**Lorentz group equivariant neural network for particle physics**." *International Conference on Machine Learning*. PMLR, 2020.

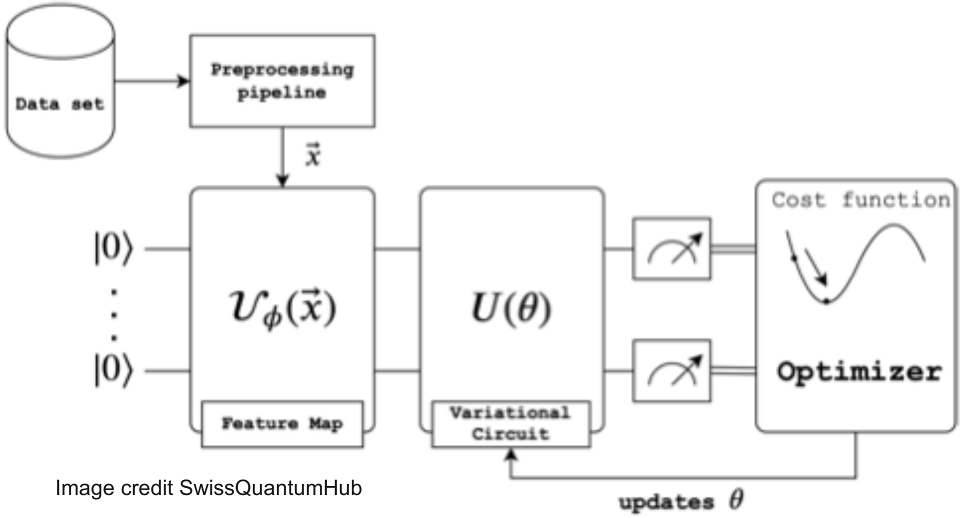


Image credit SwissQuantumHub

Kernel methods

Feature maps as **quantum kernels**

Use classical **kernel-based training**

- **Convex** losses, **global** minimum
- Compute pair-wise distances in N_{data}

Identify classes of kernels that relate to specific data **structures**[2]

2 Glick, Jennifer R., et al. "**Covariant quantum kernels for data with group structure**." *arXiv preprint arXiv:2105.03406* (2021).

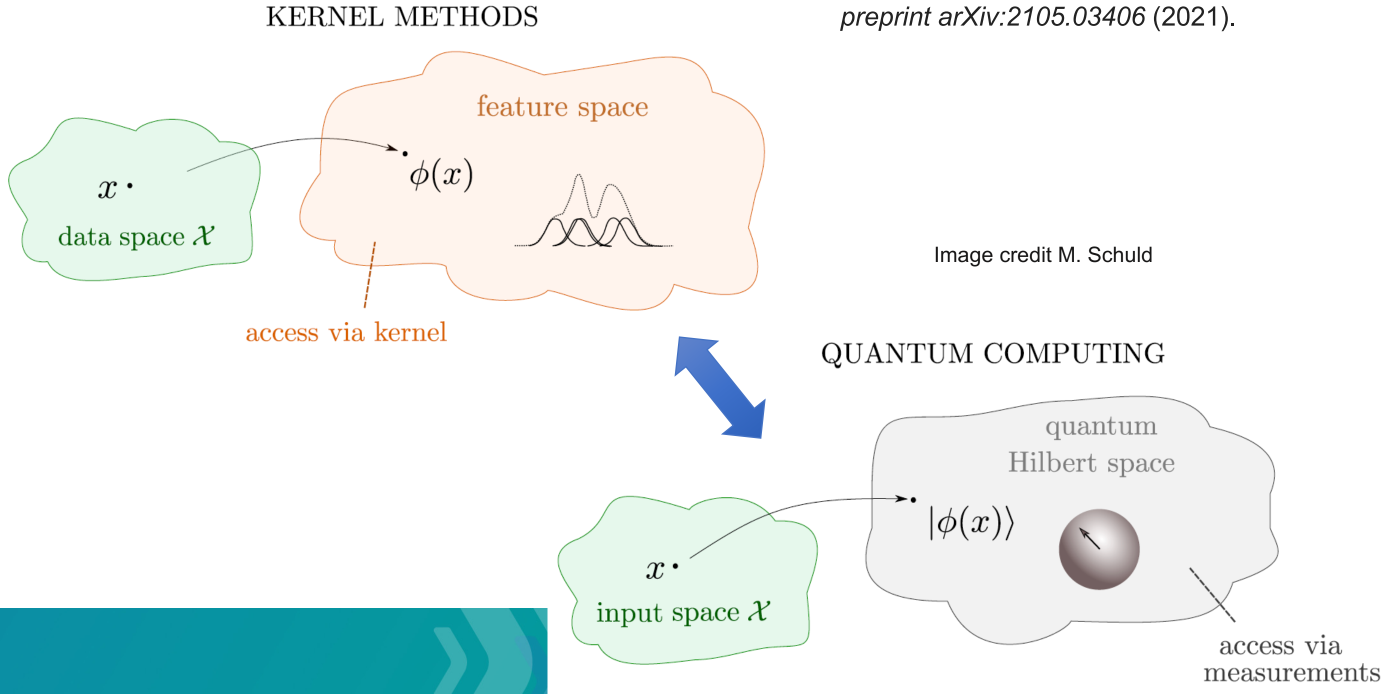


Image credit M. Schuld

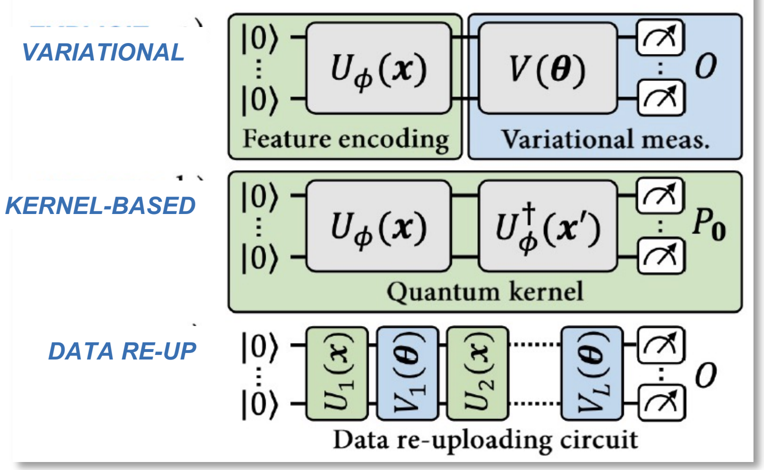
Equivalent interpretations?

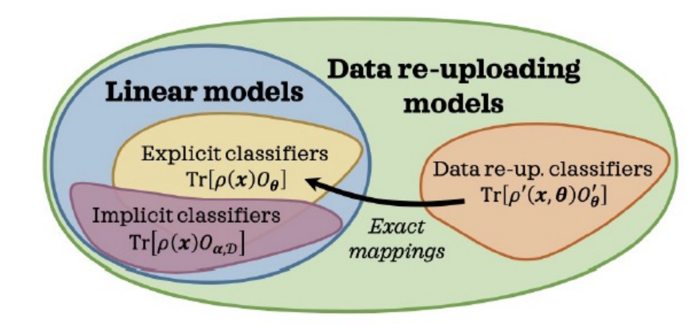
Characterize the behaviour of different architectures, **similarity and links among them** and **with the data.**

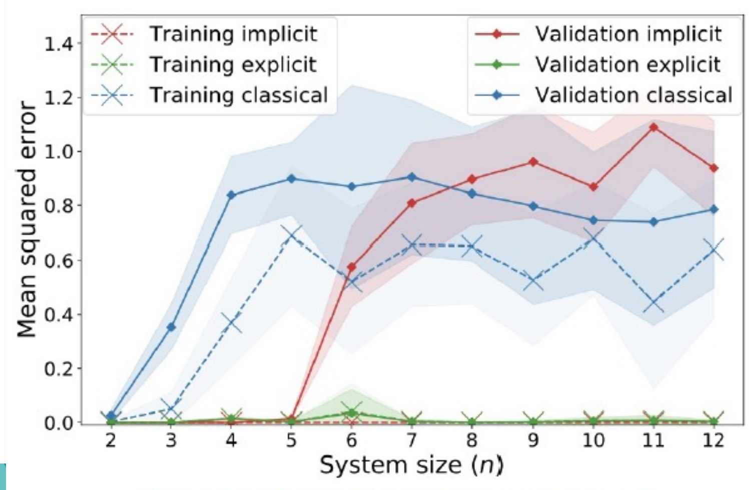
Ex:

- Data Re-Uploading circuits: alternating data encoding and variational layers.
    - Represented as **explicit linear models** (variational) in larger feature space

    → can be reformulated as **implicit models** (kernel)
- Representer theorem: implicit models achieve **better accuracy**
    - Explicit models exhibit **better generalization** performance







PCA on 28x28 fashion-MNIST dataset, ZZ feature encoding + hardware-efficient variational unitary

Jerbi, Sofiene, et al. "**Quantum machine learning beyond kernel methods.**" *arXiv preprint arXiv:2110.13162* (2021).

Model Convergence and Barren Plateau

Given the size of the Hilbert space a compromise between **expressivity**, **convergence** and **generalization** performance is needed.

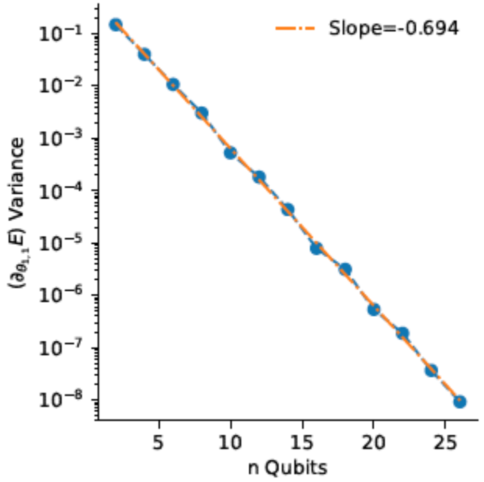
Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)

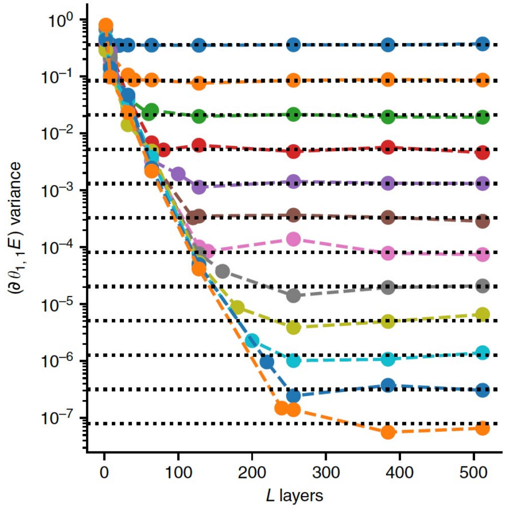
- Convergence still possible if gradients consistent between batches.

Quantum gradient decay exponentially in the number of qubits

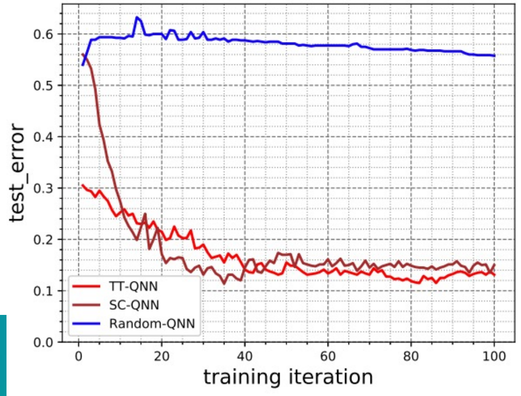
- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12,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

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

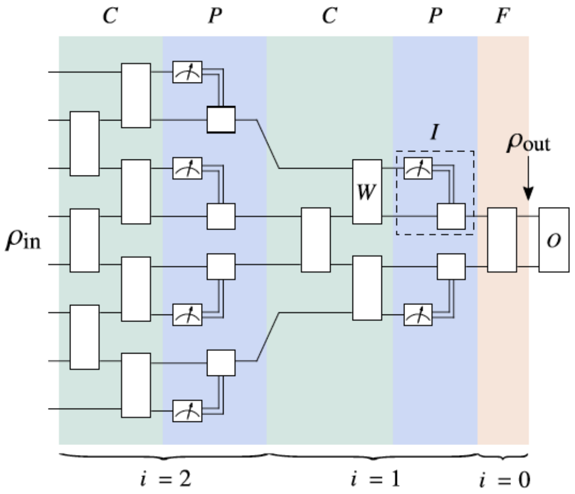




TTN for MNIST classification (8 qubits), Zhang *et al.*, arXiv:2011.06258

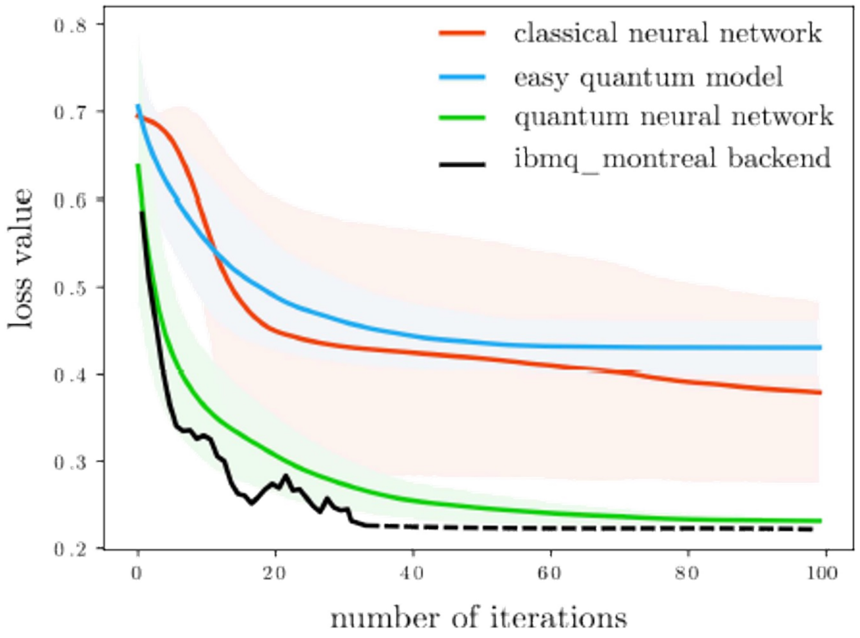


QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011



Abbas, Amira, et al. "**The power of quantum neural networks**." *Nature Computational Science* 1.6 (2021): 403-409.

Defining quantum Advantage for QML



Different possible definitions

Runtime speedup

Sample complexity

Representational power

A quantum algorithm that cannot be efficiently simulated classically

- No established recipe for classical data
- Need to use the whole exponential advantage in Hilbert space, but will it converge ?

(Algorithm expressivity vs convergence and generalization)

Kübler, Jonas, Simon Buchholz, and Bernhard Schölkopf. "**The inductive bias of quantum kernels**." Advances in Neural Information Processing Systems 34 (2021).
Huang, HY., Broughton, M., Mohseni, M. et al. **Power of data in quantum machine learning**. Nat Commun 12, 2631 (2021). https://doi.org/10.1038/s41467-021-22539-9

Practical advantage

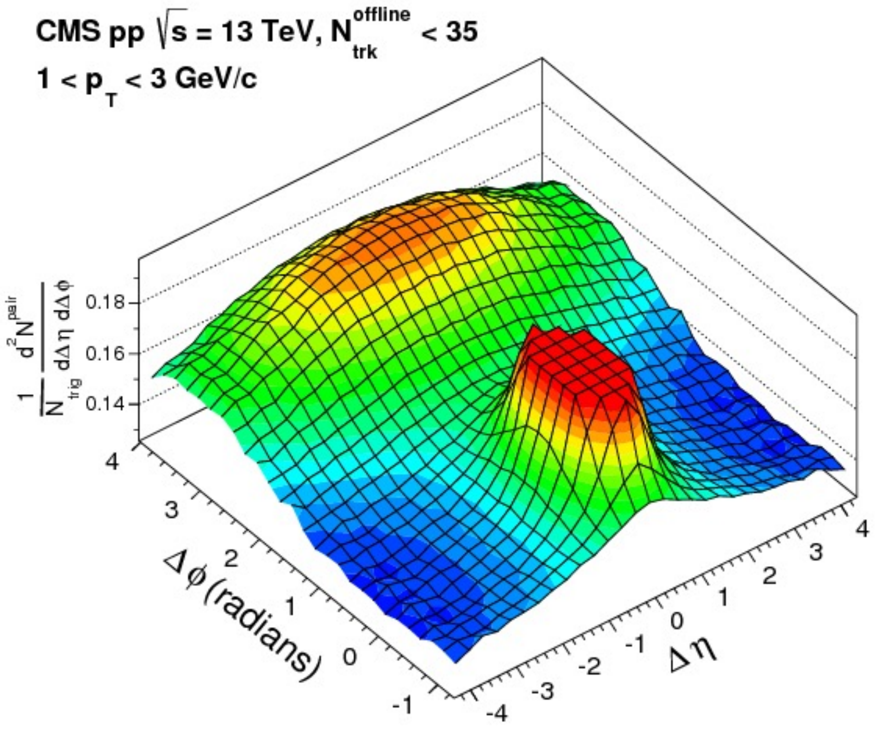
Practical implementation vs asymptotic complexity

Data embedding

NISQ vs ideal quantum devices

Realistic applications

Performance metrics and fair comparison to classical models



Khachatryan, Vardan, et al. "**Measurement of Long-Range Near-Side Two-Particle Angular Correlations in p p Collisions at s= 13 TeV**." *Physical review letters* 116.17 (2016): 172302.

HEP data is classical, but originally produced by quantum processes. It is these **intrinsically quantum correlations** we are trying to identify

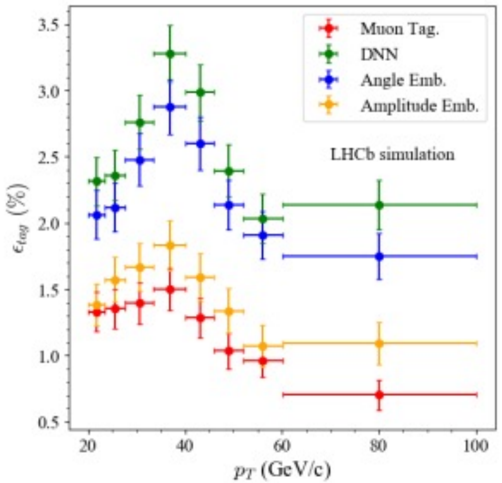
A change of paradigm could reflect in interesting insights

- What are natural building blocks for QML algorithms?
- How can we construct useful bridges between QC and learning theory?
- How can we make quantum software ready for ML applications?

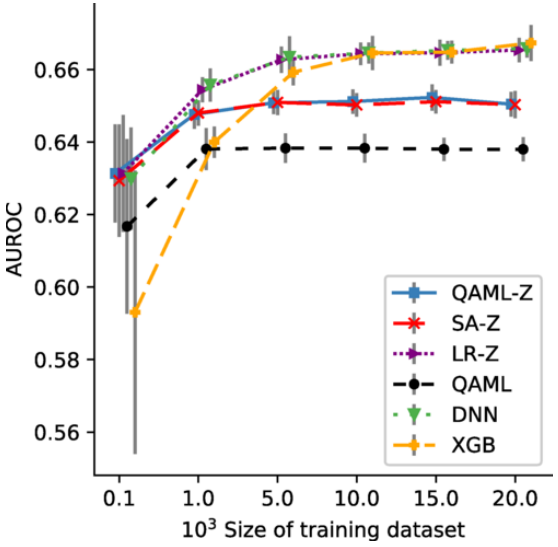
Schuld, Maria, and Nathan Killoran. "**Is quantum advantage the right goal for quantum machine learning?**." *arXiv preprint arXiv:2203.01340* (2022).

See M. Grossi summary at the 2022 CERN Openlab Technical Workshop : https://indico.cern.ch/event/1100904/contributions/4775169/

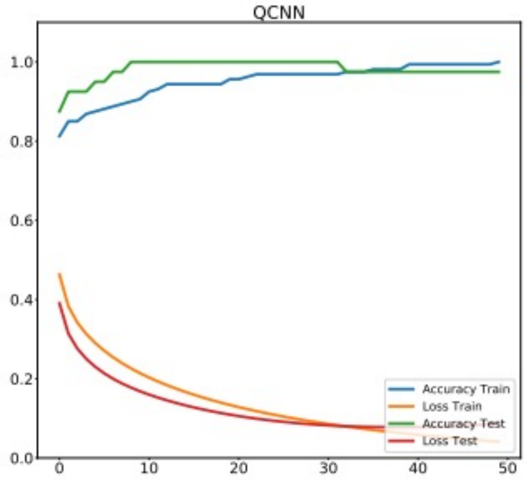
QML in High Energy Physics



Alexander Zlokapa, Alex Mott, Joshua Job, Jean-Roch Vlimant, Daniel Lidar, and Maria Spiropulu. **Quantum adiabatic machine learning by zooming into a region of the energy surface.** Physical Review A, 102:062405, 2020. DOI:10.1103/PhysRevA.102.062405.

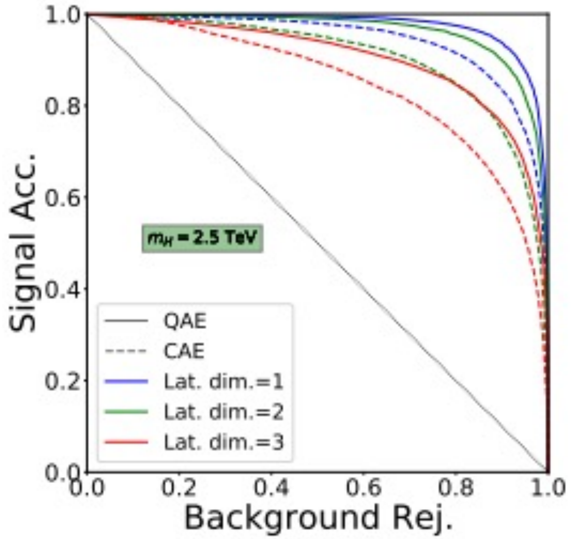


Samuel Yen-Chi Chen, Tzu-Chieh Wei, Chao Zhang, Haiwang Yu, and Shinjae Yoo. **Quantum convolutional neural networks for high energy physics data analysis.** arXiv preprint: 2012.12177, 2020.

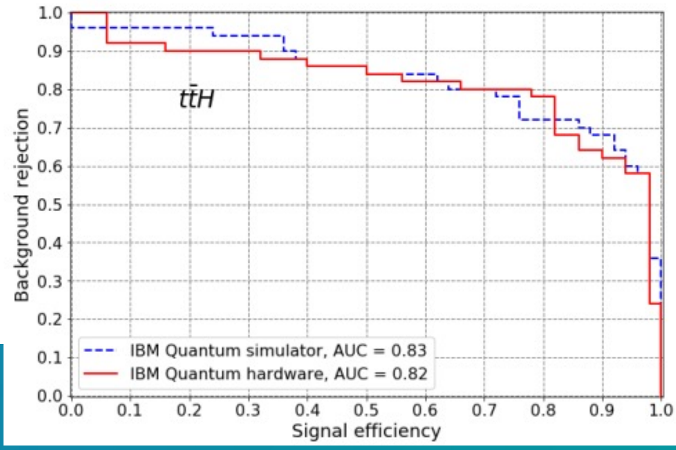


Alessio Gianelle, Patrick Koppenburg, Donatella Lucchesi, Davide Nicotra, Eduardo Rodrigues, Lorenzo Sestini, Jacco de Vries, and Davide Zuliani. **Quantum Machine Learning for *b*-jet identification.** arXiv:2202.13943, 2022.

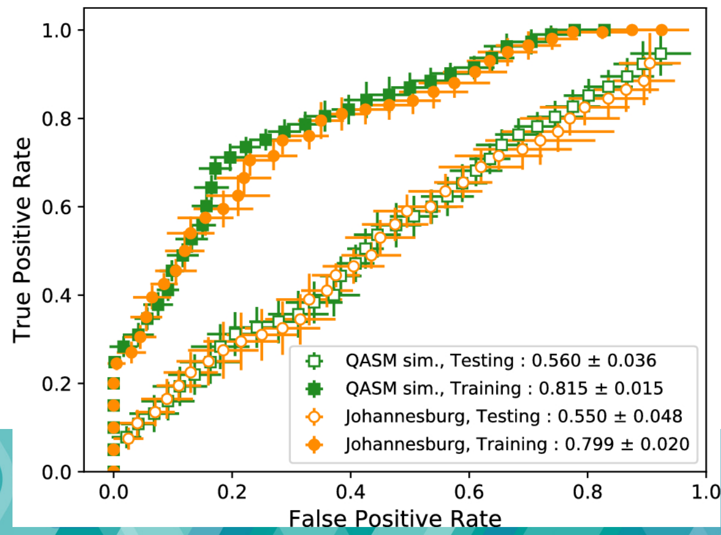
Vishal S Ngairangbam, Michael Spannowsky, and Michihisa Takeuchi. **Anomaly detection in high-energy physics using a quantum autoencoder**. arXiv preprint arXiv:2112.04958, 2021.



Sau Lan Wu, Jay Chan, Wen Guan, Shaojun Sun, Alex Wang, Chen Zhou, Miron Livny, Federico Carminati, Alberto Di Meglio, Andy C Y Li, and et al. **Application of quantum machine learning using the quantum variational classifier method to high energy physics analysis at the lhc on ibm quantum computer simulator and hardware with 10 qubits**. Journal of Physics G: Nuclear and Particle Physics, 48(12):125003, Oct 2021

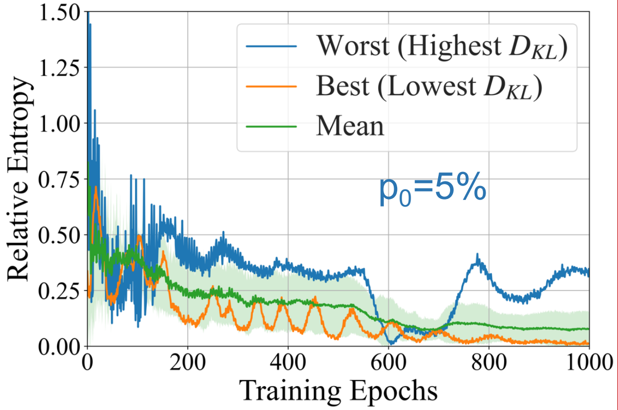


Koji Terashi, Michiru Kaneda, Tomoe Kishimoto, Masahiko Saito, Ryu Sawada, and Junichi Tanaka. **Event classification with quantum machine learning in 20 high-energy physics**. Computing and Software for Big Science, 5(1), January 2021.

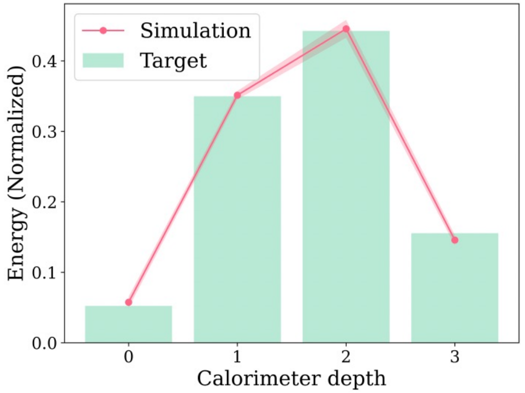


QML at CERN

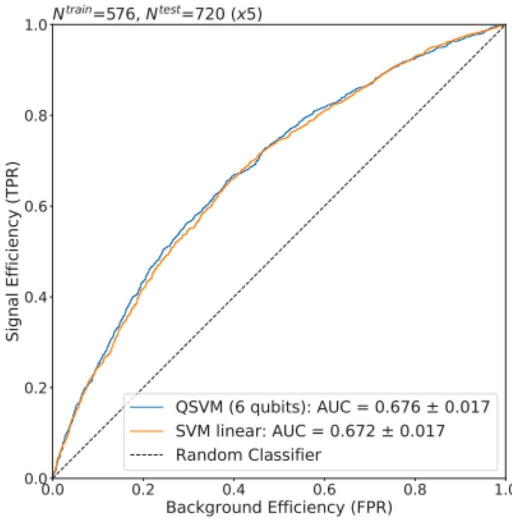
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." *arXiv preprint arXiv:2203.01007* (2022).



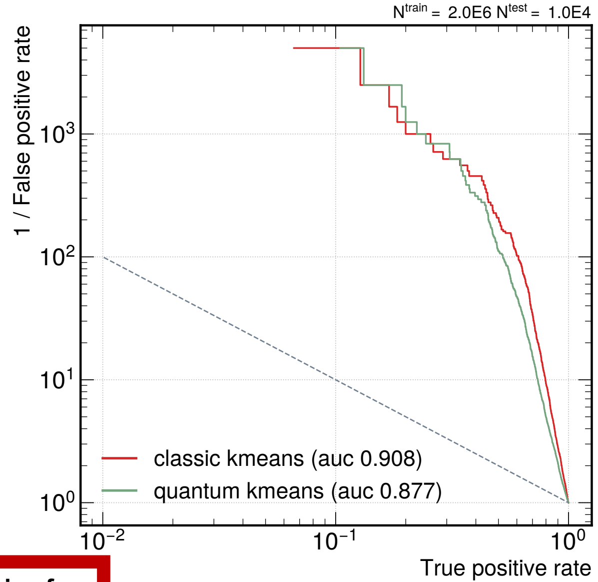
Chang S.Y. *et al.,* **Running the Dual-PQC GAN on Noisy Simulators and Real Quantum Hardware**, QTML2021, ACAT21



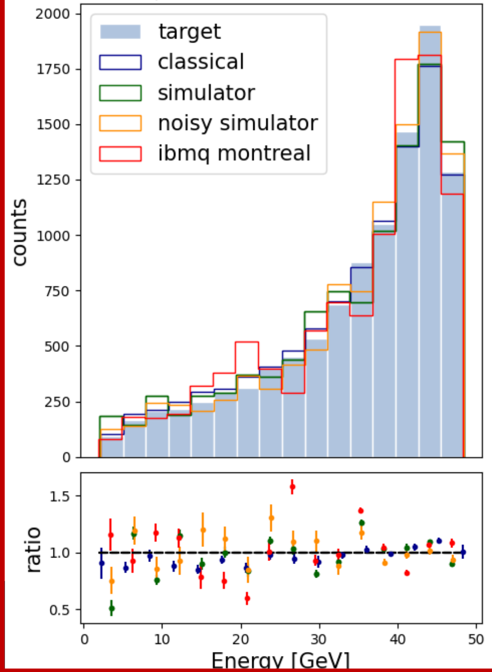
Vasilis Belis, Samuel González-Castillo, Christina Reissel, Sofia Vallecorsa, Elías F. Combarro, Günther Dissertori, and Florentin Reiter. **Higgs analysis with quantum classifi**ers. EPJ Web of Conferences, 251:03070, 2021



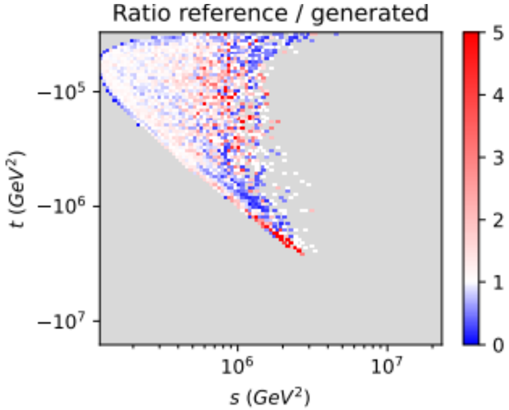
Kinga Wozniak, **Unsupervised clsutering for a Randall–Sundrum Graviton at 3.5TeV narrow resonance**



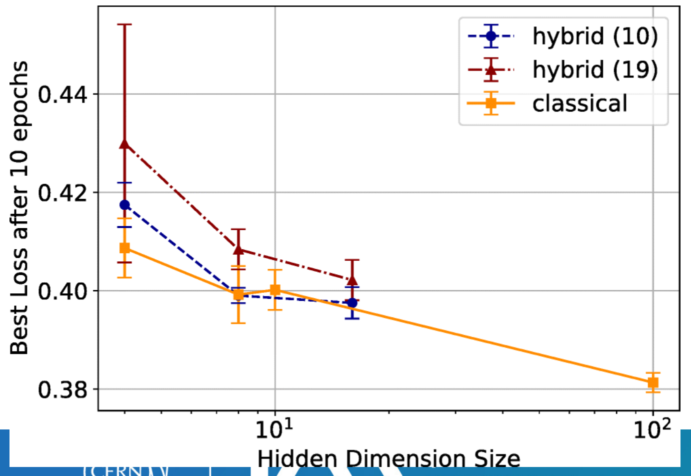
O. Kiss, **Quantum Born Machine for event generation**, ACAT2021



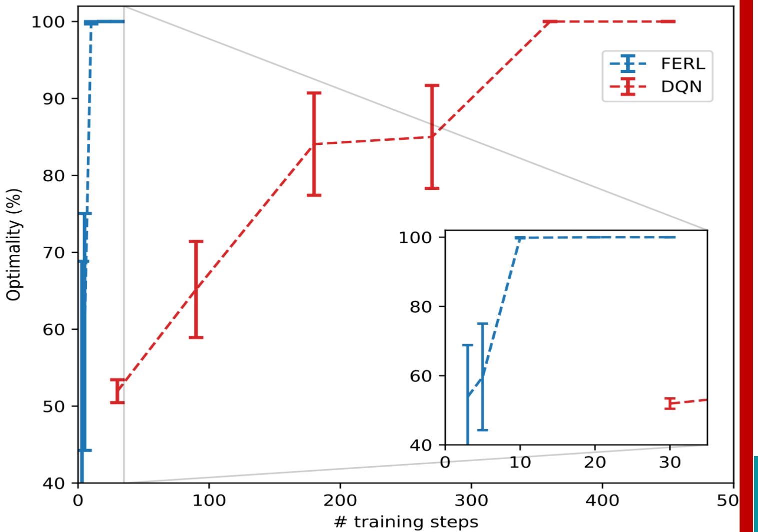
Bravo-Prieto, Carlos, et al. "**Style-based quantum generative adversarial networks for Monte Carlo events**." *arXiv preprint arXiv:2110.06933* (2021).



Tüysüz, Cenk, et al. "**Hybrid quantum classical graph neural networks for particle track reconstruction**." *Quantum Machine Intelligence* 3.2 (2021): 1-20.



M. Shenk, V. Kain, **Quantum Reinformcement Learning**, BQiT 2021, 2022 CERN openlab Tech Workshop

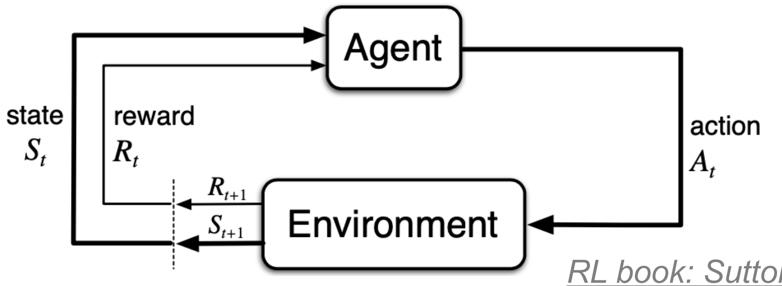


M. Shenk, V. Kain
BQiT 2021
2022 CERN openlab Tech Workshop

Quantum Reinforcement Learning

Q-learning – learn value function Q(s, a) using **function approximator**

- **DQN: Deep Q-learning** *(feed-forward neural network)*
- **QBM-RL** *(Quantum Boltzmann Machine)*



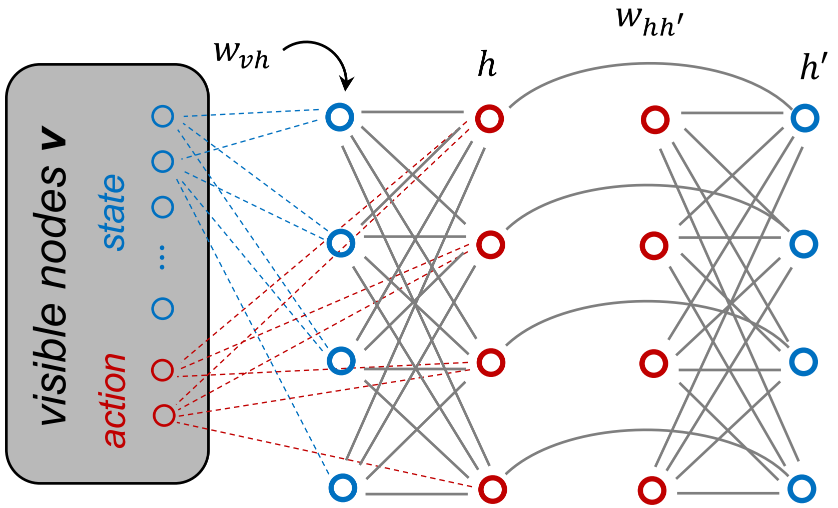
RL book: Sutton & Barto

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

Free Energy RL: clamped QBM

- **Network of coupled, stochastic, binary units** (spin up / down)
- $\hat{\boldsymbol{Q}}(\boldsymbol{s},\boldsymbol{a})$ **≈ 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

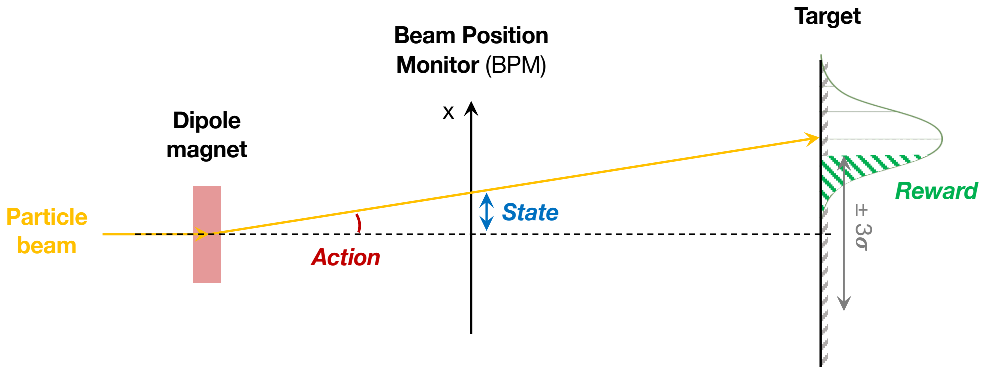
Clamped QBM



M. Schenk
2022 CERN openlab technical workshop

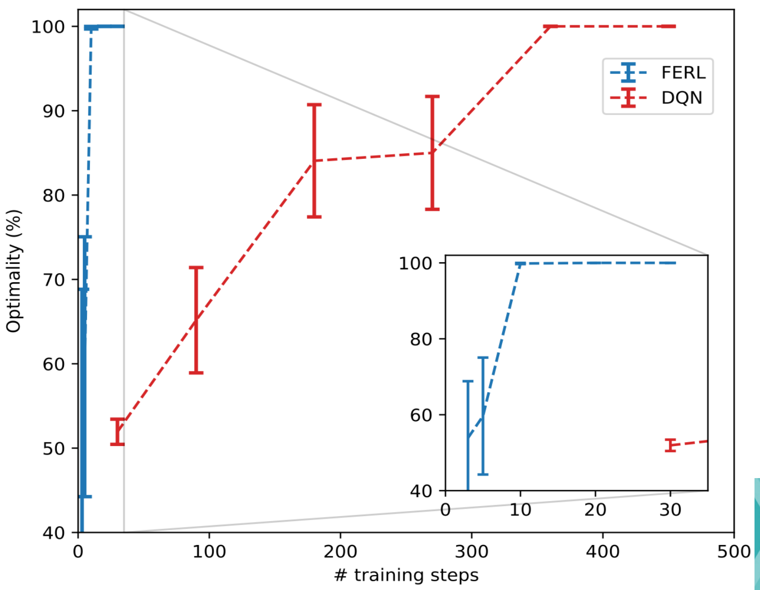
Beam optimisation in linear accelerator

- **Action: deflection** angle
- **State: BPM** position
- **Reward: integrated beam intensity on target**
- **Optimality**: what fraction of possible states does agent take the right decision

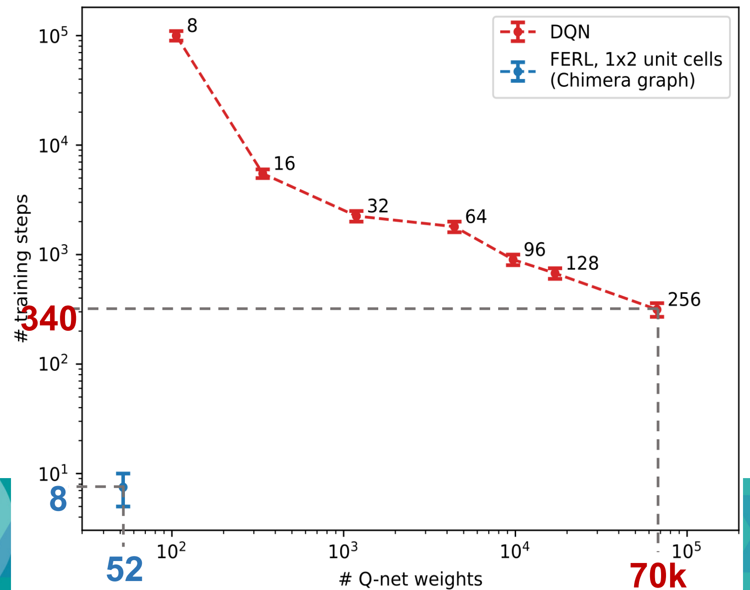


- **Training efficiency:** FERL **massively** outperforms classical Q-learning *(8±2 vs. 320±40 steps)*
- **Descriptive power:** QBM can reach high performance with **much fewer weights** than DQN *(52 vs. ~70k)*

Training efficiency



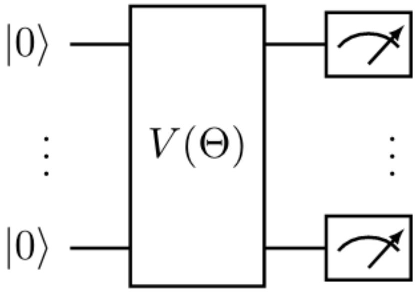
Training efficiency vs. # Q-net / QBM weights



Quantum Circuit Born Machine

Sample from a variational wavefunction $|\psi(\theta)\rangle$ with probability given by the **Born rule**:

$$p_\theta(x) = |\langle x|\psi(\theta)\rangle|^2$$



- Only able to generate **discrete PDFs** (continuous in the limit #qubits $\rightarrow \infty$)
- Train using **Maximum Mean Discrepancy**:

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

with K a gaussian kernel

- **Pros**: relativly easy to optimize, **Cons**: empircally less efficient than an adversarial approach

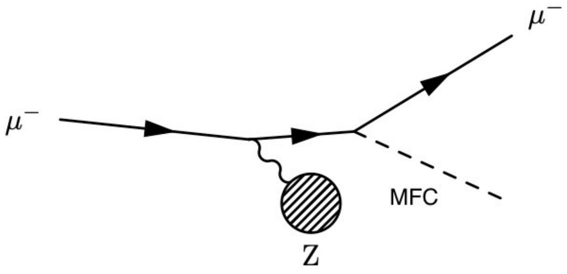
Coyle, B., Mills, D. et al, **The Born supremacy.** In: *npj Quantum Inf 6, 60* (2020)

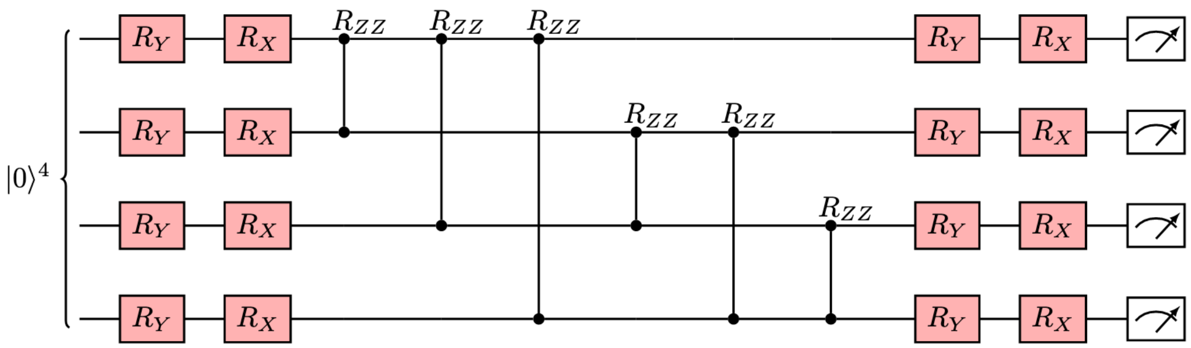
QCBM for event generation

Muon Force Carriers predicted by several theoretical models:

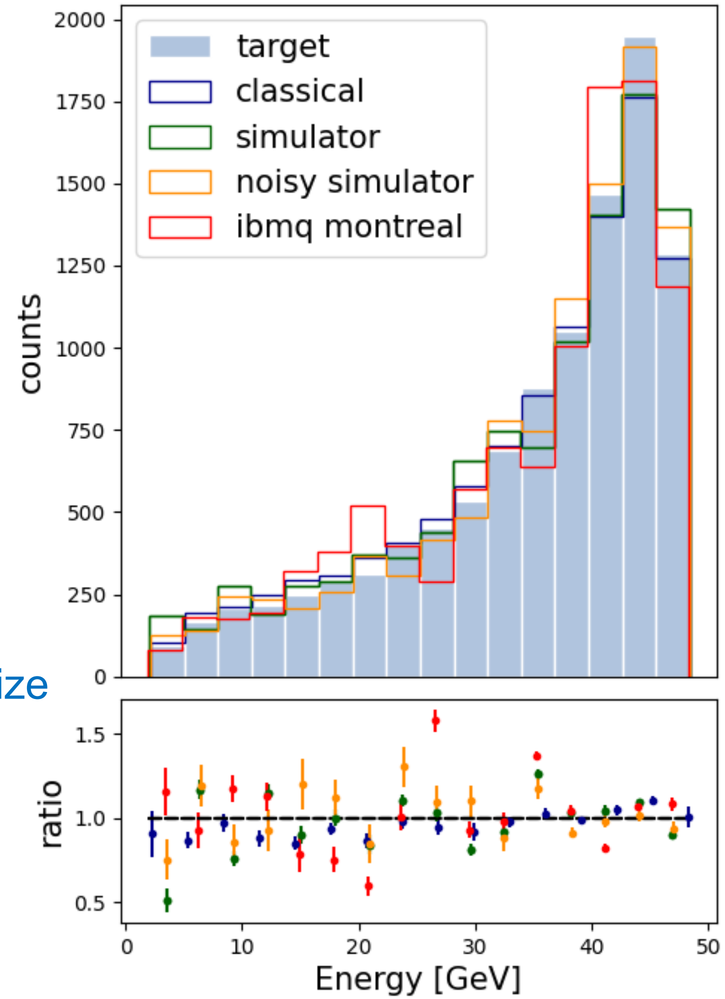
- Could be detected by muon fixed-target experiments (FASER) or muon interactions in calorimeters (ATLAS)[1].

Generate E, p_t, η of outgoing muon and MFC





Perfect simulator
Noisy simulator (IBMQ casablanca) (no error mitigation)
IBMQ Montreal
Classical GMMD of size (15,128, 256,128,16,1)
Easy GMMD ~ QCBM in size

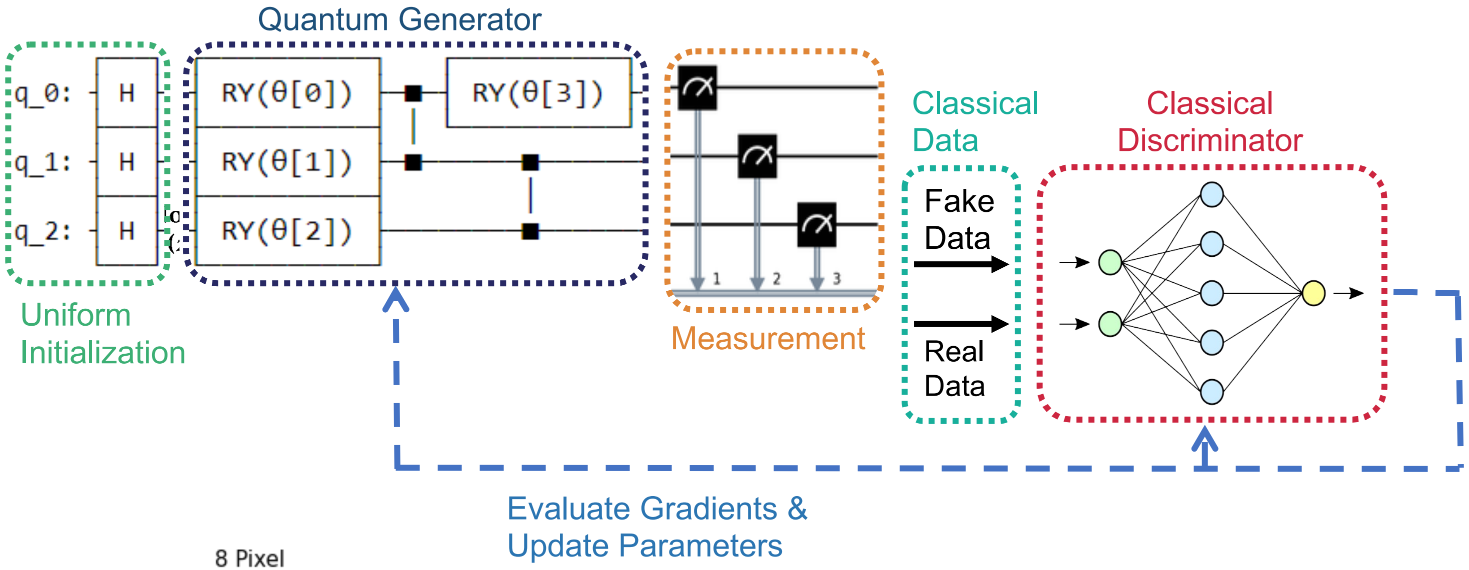


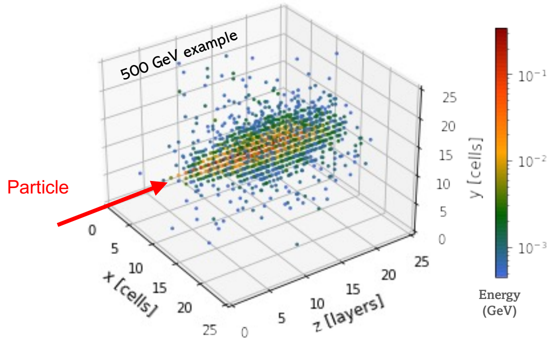
1 Galon, I, Kajamovitz, E et al. "Searching for muonic forces with the ATLAS detector". In: Phys. Rev. D 101, 011701 (2020)

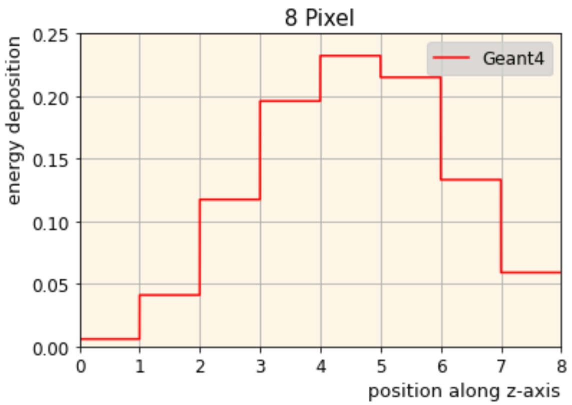
Quantum Generative Adversarial Networks

Generating Energy Profiles in Calorimeters

- Single particles generate energy deposits in a calorimeter
- Represented as a 3D regular grid
- Reduce to:
- 1D distribution along the calorimeter depth
- 2D distribution on the y-z plane







Borras, Kerstin, et al. "Impact of quantum noise on the training of quantum Generative Adversarial Networks." *arXiv preprint arXiv:2203.01007* (2022).

Rehm, Florian, et al. "Quantum Machine Learning for HEP Detector Simulations." (2021).

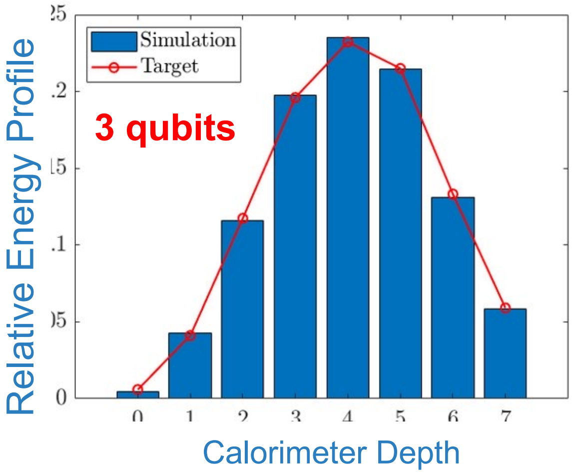
Quantum generation of energy profiles

IBM qGAN[1] can load probability distributions in quantum states

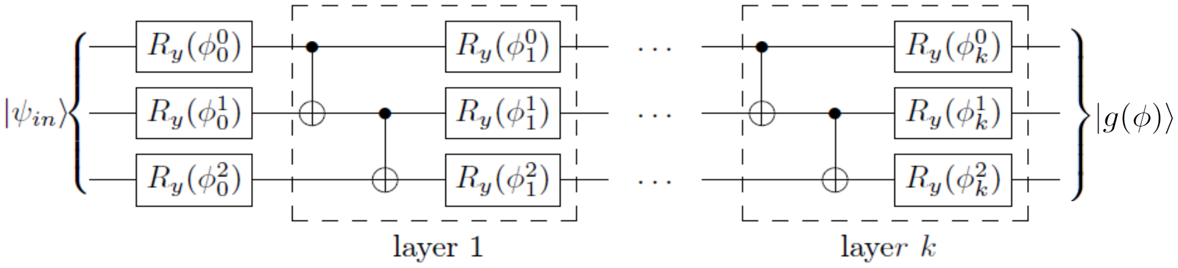
Simplify simulation problem

1D & 2D energy profiles from detector

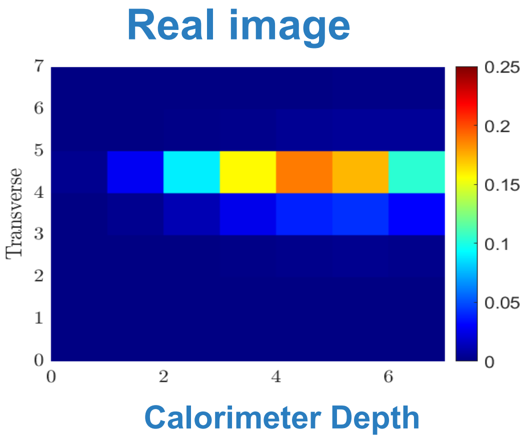
Train a **hybrid classical-quantum** GAN to generate **average image**

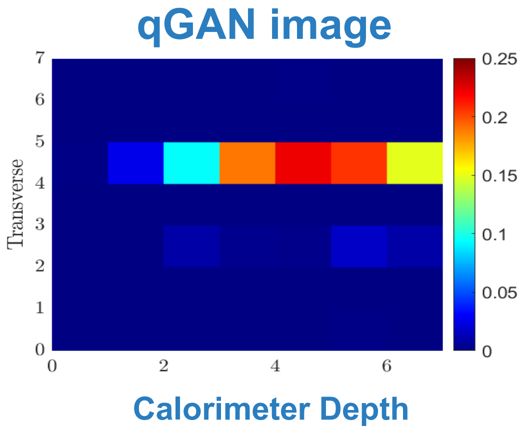


Quantum Generator: 3 R_y layers



6 qubits



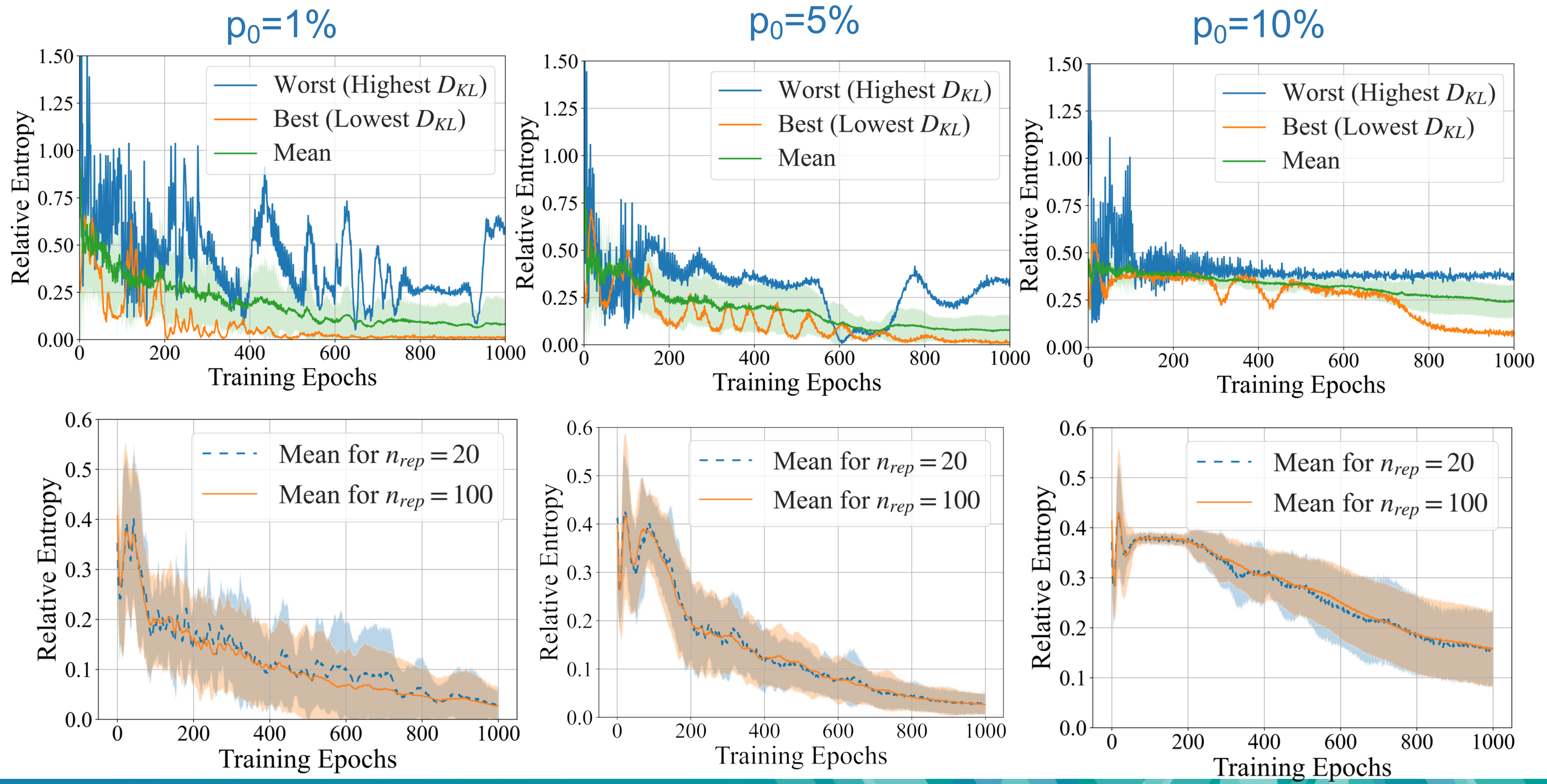


1 Zoufal, C., Lucchi, A. & Woerner, S. Quantum Generative Adversarial Networks for learning and loading random distributions. *npj Quantum Inf* **5,** 103 (2019). https://doi.org/10.1038/s41534-019-0223-2

Borras, Kerstin, et al. "Impact of quantum noise on the training of quantum Generative Adversarial Networks." *arXiv preprint arXiv:2203.01007* (2022).

Readout noise effect on GAN training

- Training is up to ~5% readout **noise tolerant**
- **Higher readout noise reduces** accuracy
- **Intrinsic instability** in the training process

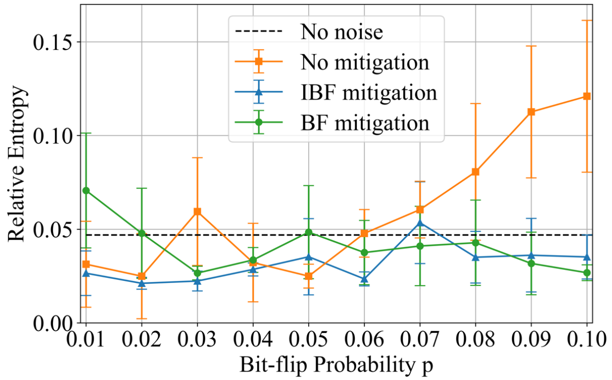


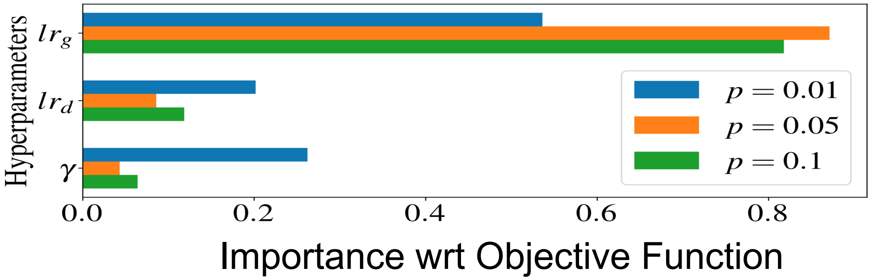
Running the model on noisy devices

Florian Rehm, S. Y. Chang:
https://arxiv.org/abs/2203.01007

Train on noisy simulator

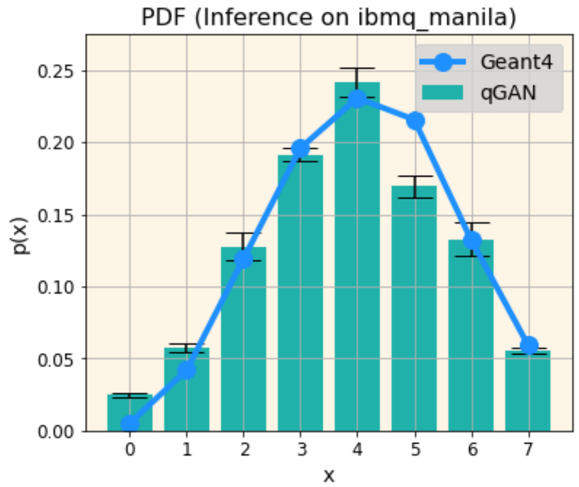
- Evaluate importance of training hyperparameters
- **Error mitigation needed only** for **higher** noise level

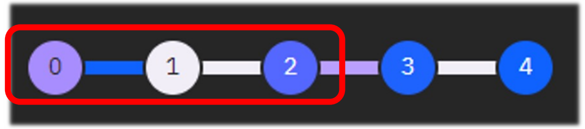




Inference on IBM Q Manila hardware

- Maintain good physics perfomance





Qubit Number	0	1	2
Readout Error	2.34%	2.66%	2.05%
CX-gate Error	1.11%		1.75%

Summary

Research on QML applications in High Energy Physics is producing a large number of prototypes

- So far focus on different steps of data processing in «controlled environment»
- Some **preliminary hints** of advantage in terms of input feature size and representational power
- Mostly we do «**as good as classical methods**»
- Need **more robust studies** to relate quantum model architecture and performance to data sets
- Identify use cases where **quantum approach** could be **more effective** than classical machine/deep learning
- Studying QML algorithms today can build links between **QC and learning theory**

Thanks!

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