# Quantum Computing at CERN

QUANTUM TECHNOLOGY INITIATIVE

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AI and Quantum Research - CERN openlab

CERN

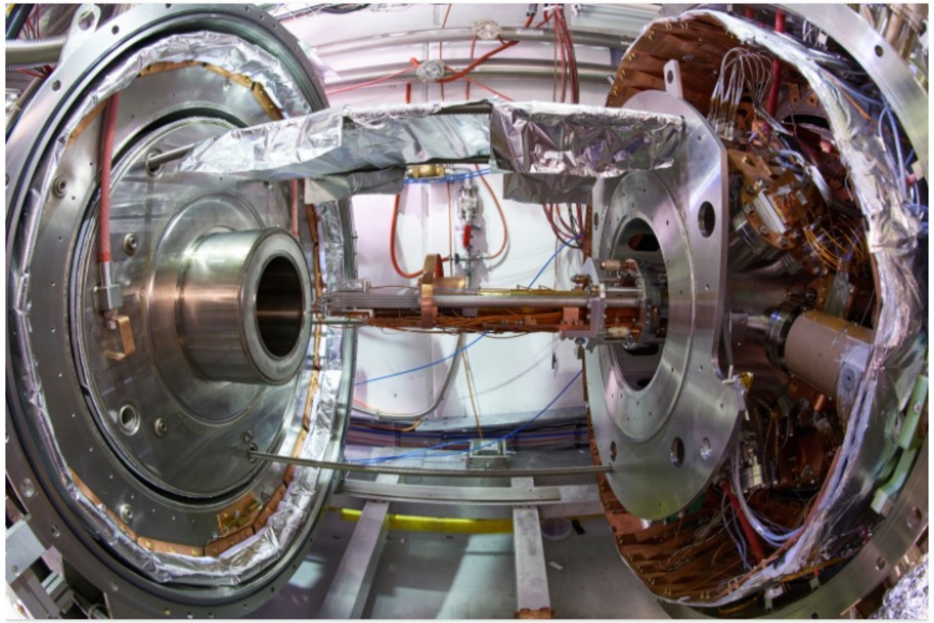
# CERN QTI and its Roadmap

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)

## 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

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

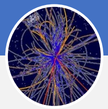
Credit: CERN

T3 - Community Building

T4 - Integration with national and international initiatives and programmes

INITIATIVE

# Scientific Objectives



## Computing & Algorithms

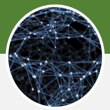
- Assess the **areas of potential quantum advantage** in HEP (QML, classification, anomaly detection, tracking)
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

## Simulation & Theory

- 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

## Sensing, Metrology & Materials

- 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



## Communications & Networks

- **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)

# 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 Advantage?

https://www.nature.com/articles/s41586-019-1666-5


In 2019, **Google** claimed quantum advantage by solving a sampling problem: 200s on Sycamore vs  estimated 10k years on Summit
In 2020, **Hefei National Lab, China**, measured advantage on another sampling using a photonic computer

**Quantum supremacy** refers to quantum computers that ".. can do things that classical computers can't, **regardless of whether those tasks are useful.**"  (**John Preskill, Caltech**)

**Practical quantum advantage**
"Solve a problem that is useful either for academia or industry **faster or better than any known classical algorithm** on the best classical computer" (**M. Troyer, Microsoft**)

arXiv:2005.06787v1 [quant-ph] 14 May 2020

Classical Simulation of Quantum Supremacy Circuits

Cupjin Huang,[1] Fang Zhang,[2] Michael Newman,[3] Junjie Cai,[4] Xun Gao,[1] Zhengxiong Tian,[5] Junyin Wu,[4] Haihong Xu,[5] Huanjun Yu,[5] Bo Yuan,[6] Mario Szegedy,[1] Yaoyun Shi[1], Jianxin Chen[1]

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[2]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109, USA
[3]Departments of Physics and Electrical and Computer Engineering, Duke University, Durham, NC 27708, USA
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[6]Alibaba Infrastructure Service, Alibaba Group, Hangzhou, Zhejiang 310000, China

Abstract

It is believed that random quantum circuits are difficult to simulate classically. These have been used to demonstrate quantum supremacy: the execution of a computational task on a quantum computer that is infeasible for any classical computer. The task underlying the assertion of quantum supremacy by Arute *et al.* (*Nature*, **574**, 505–510 (2019)) was initially estimated to require Summit, the world's most powerful supercomputer today, approximately 10,000 years. The same task was performed on the Sycamore quantum processor in only 200 seconds.

In this work, we present a tensor network-based classical simulation algorithm. Using a Summit-comparable cluster, we estimate that our simulator can perform this task in less than 20 days. On moderately-sized instances, we reduce the runtime from years to minutes, running several times faster than Sycamore itself. These estimates are based on explicit simulations of parallel subtasks, and leave no room for hidden costs. The simulator's key ingredient is identifying and optimizing the "stem" of the computation: a sequence of pair-

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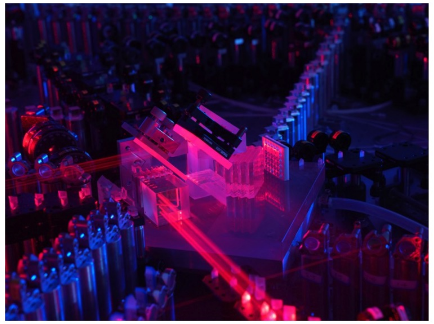
NEWS | 03 December 2020

**Physicists in China challenge Google's 'quantum advantage'**

Photon-based quantum computer does a calculation that ordinary computers might never be able to do.

Philip Ball



This photonic computer performed in 200 seconds a calculation that on an ordinary supercomputer would take 2.5 billion years to complete. Credit: Hansen Zhong

https://www.nature.com/articles/d41586-020-03434-7

# Quantum promise…

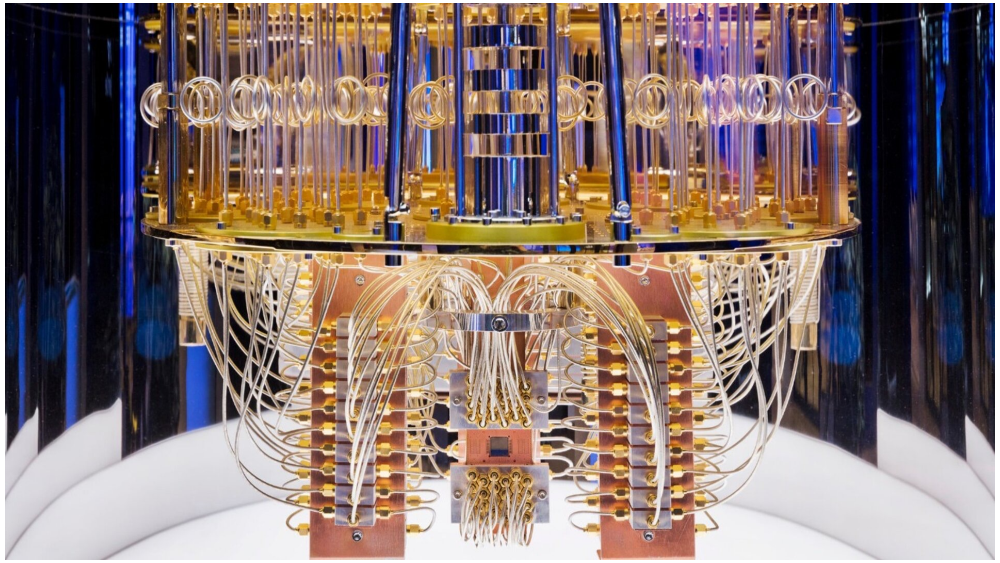
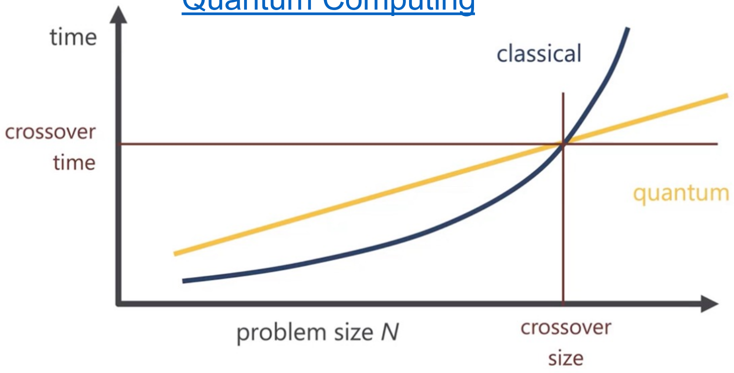


Image: IBM Q

- Exponential speedup on complex algorithms
  - Efficient **sampling**, **searches** and **optimization**
  - Linear algebra, matrices and machine learning
- New algorithms/methods for **cryptography** and **communication**
- **Direct simulation** of quantum systems

[Complexity and Quantum Computing]



# … and the challenges

- **Noisy Intermediate-Scale Quantum** devices
  - Limitations in terms of **stability** and **connectivity**
  - **De-coherence**, measurement errors or gate level errors (**noise**)
    - Need specific **error mitigation techniques**
    - **Circuit optimisation**
    - Prefer algorithms that are more **robust against noise** (variational approaches, quantum machine learning, …)
- Quantum computers initially integrated in **hybrid quantum-classical infrastructure**
  - Engineering, cooling, I/O
  - Hybrid algorithms, QPU as accelerators

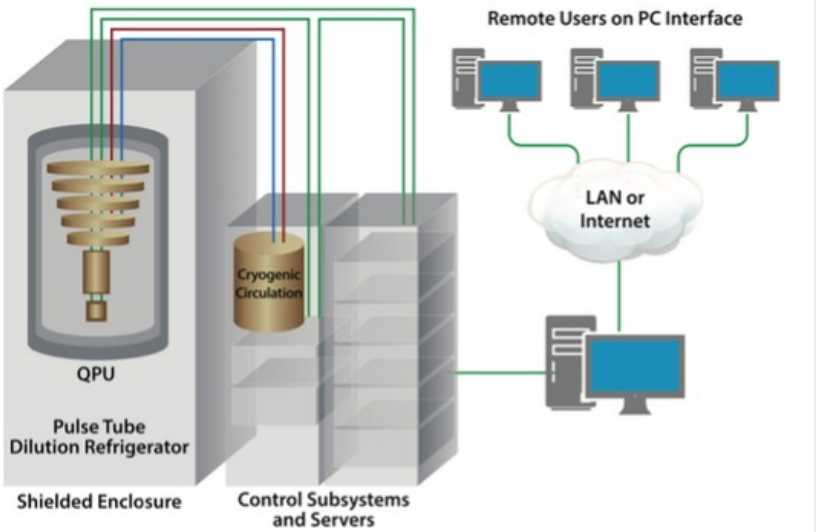
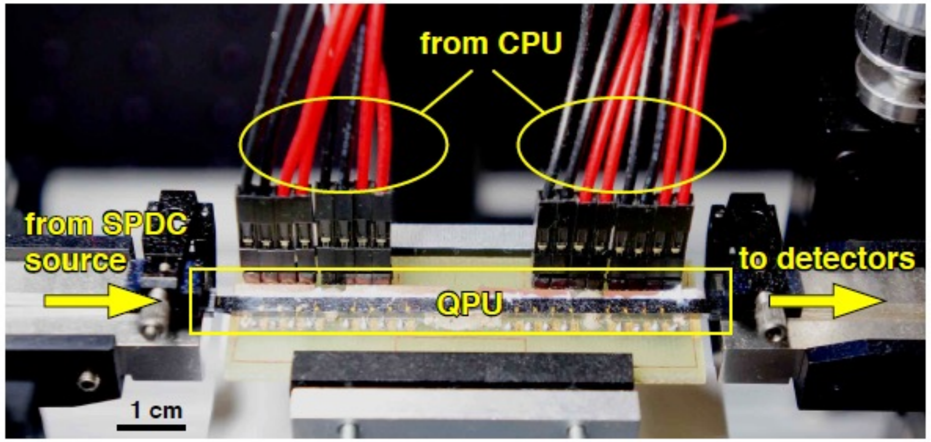



Image: D-Wave tutorial

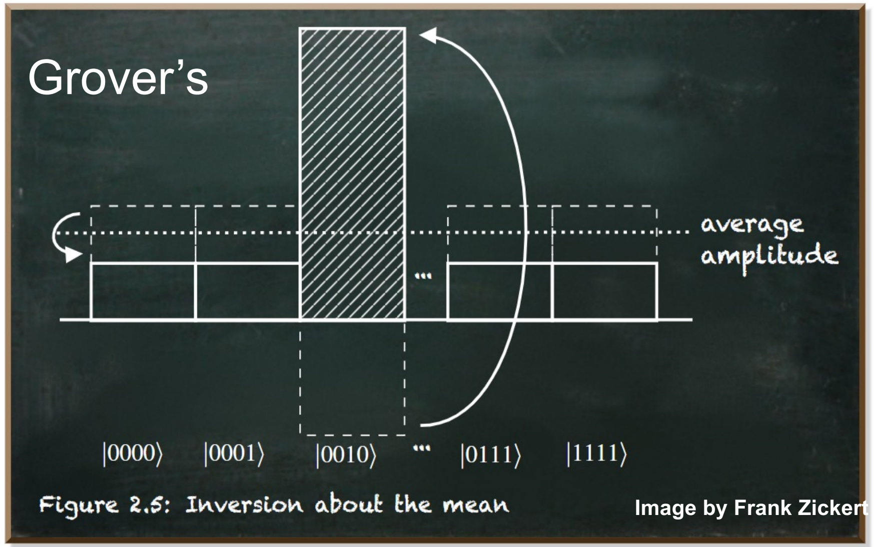
Peruzzo, A. "A variational eigenvalue solver on a quantum processor. eprint." *arXiv preprint arXiv:1304.3061* (2013).

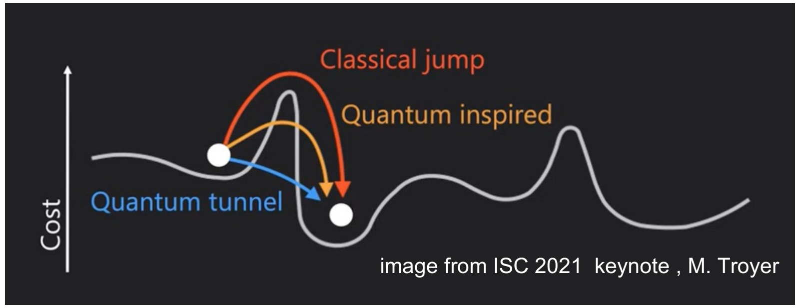


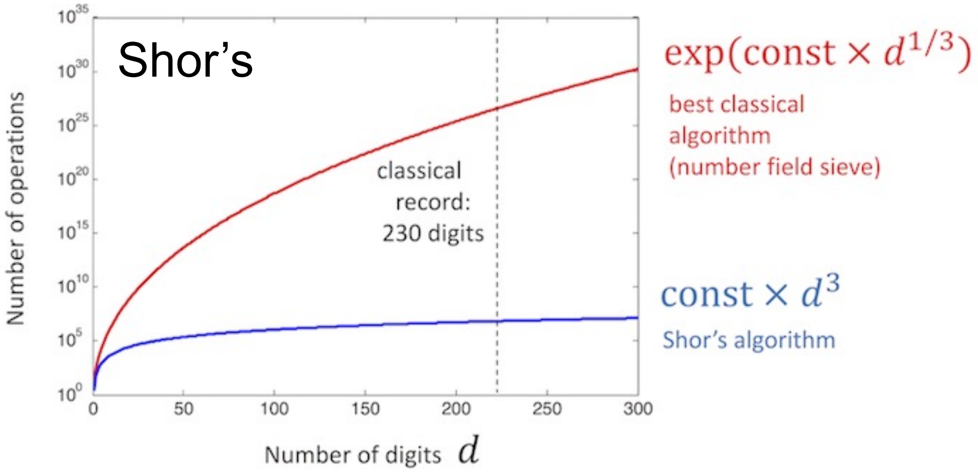
# Quantum Algorithms

A collection on **http://quantumalgorithmzoo.org**

- Multiple algorithms have been studied
  - Shor algorithm for **prime factorization**
  - Grover algorithm for unsorted DB **searches**
  - Quantum **Fourier Transform**
  - …
- Quantum-inspired algorithms (emulate quantum effects on classical hardware)
- Quantum Machine Learning
- Challenge is re-thinking **algorithms design** and define fair **benchmarking** and **comparison** to classical algorithms




https://quantum-computing.ibm.com/composer/docs/iqx/guide/shors-algorithm

# Quantum Machine Learning

Quantum circuits are **differentiable** and can be trained **minimizing a cost function** that depends on the training data

Use **Quantum Computing** to accelerate **ML/DL.** Need to address several points:

1. **Feature extraction** and **data encoding**
   - How do we represent classical data in quantum states?
2. **Model definition** (kernel based or variational)
   - The role of non-linearities?
   - Choice wrt data
3. **Optimisation** and **convergence**
   - How to reach convergence in the Hilbert space
   - Barren plateau and vanishing gradients
   - Gradient-free or gradient-based optimisers
   - (Back-propagation, automatic differentiation,..)
   - …

Different tools can enable hybrid computations

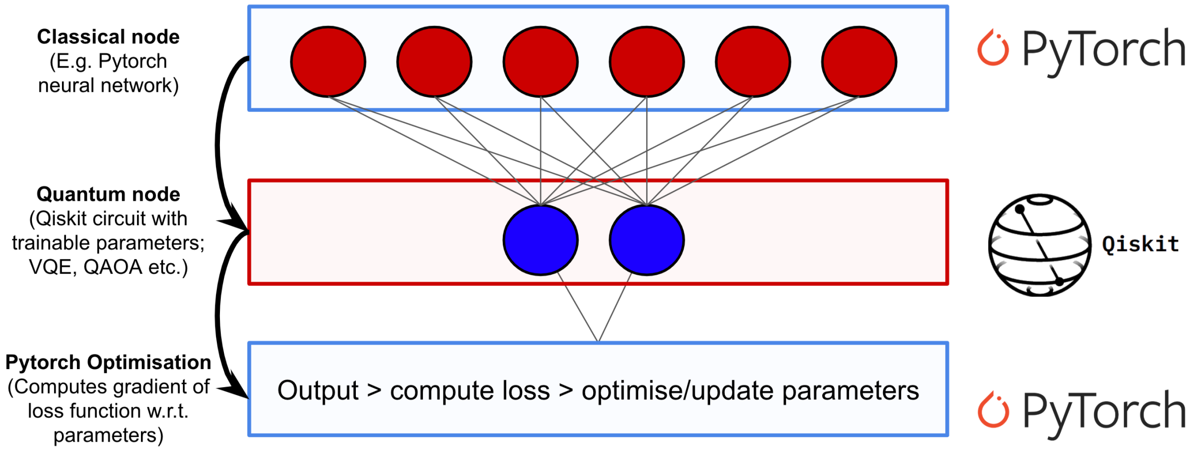
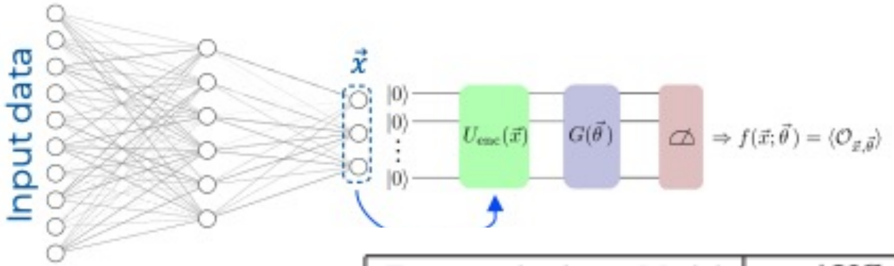



Image credit Qiskit.org/textbook

# Dimensionality reduction and data embedding




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

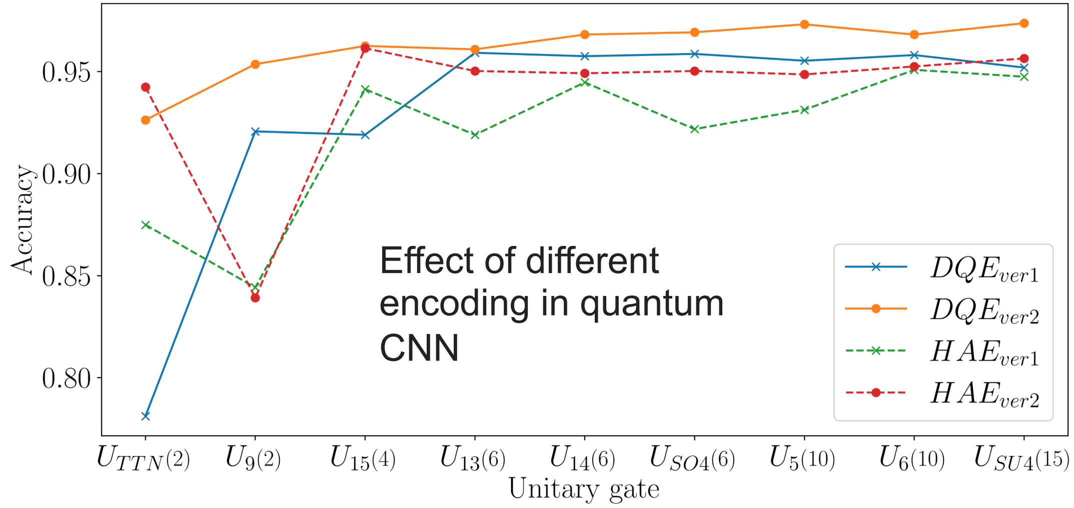
| Feature selection + Model | AUC |
|---|---|
| AUC + QSVM | $0.66 \pm 0.01$ |
| PyTorch AE + QSVM | $0.62 \pm 0.03$ |
| AUC + SVM rbf | $0.65 \pm 0.01$ |
| PyTorch AE + SVM rbf | $0.62 \pm 0.02$ |
| KMeans + SVM rbf | $0.61 \pm 0.02$ |

**Dimensionality reduction/feature extraction**

- Reduce size of classical data and optimize input features for specific tasks (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)




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.

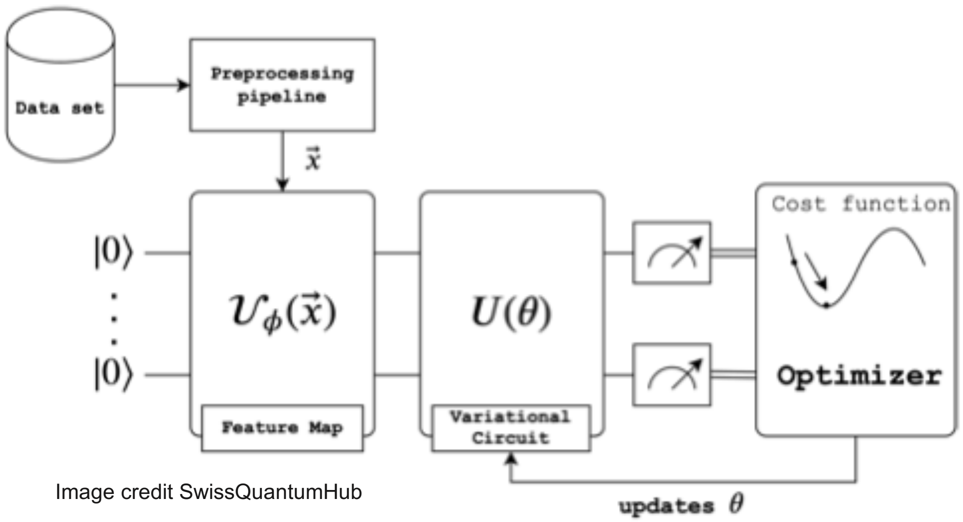



Image credit SwissQuantumHub

## *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).

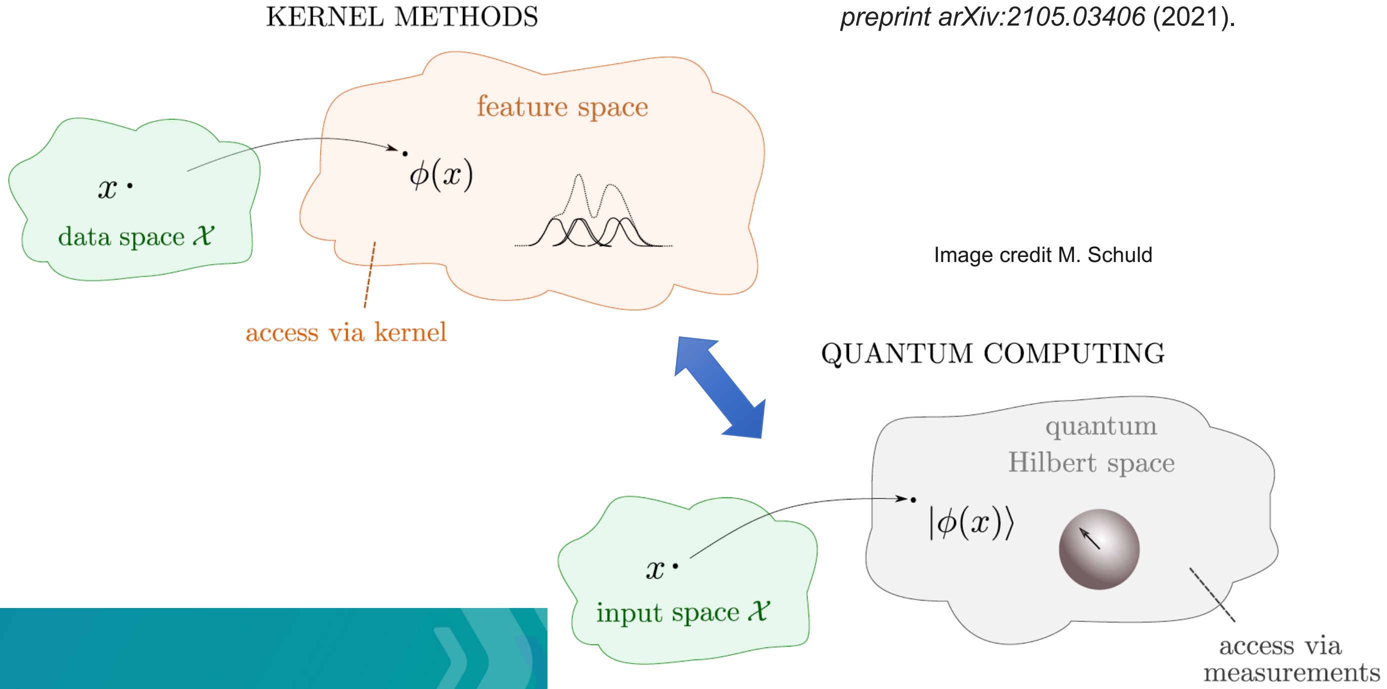



Image credit M. Schuld

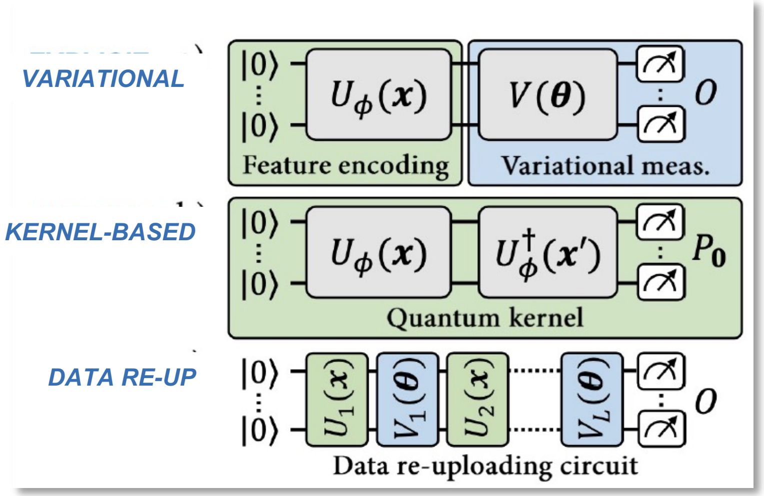
# Equivalent interpretations

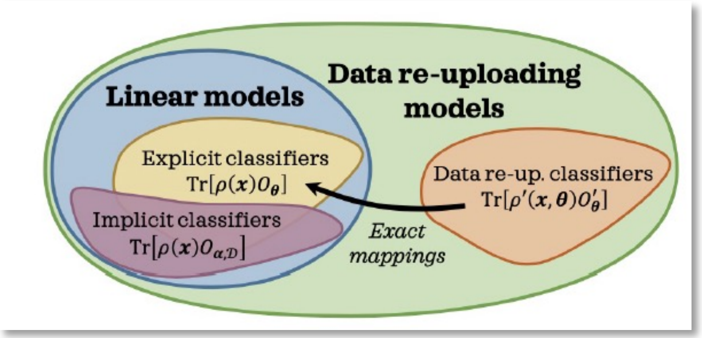
**Important to characterize the behaviour** of different architectures, **similarity and links among them** and **with the data.**

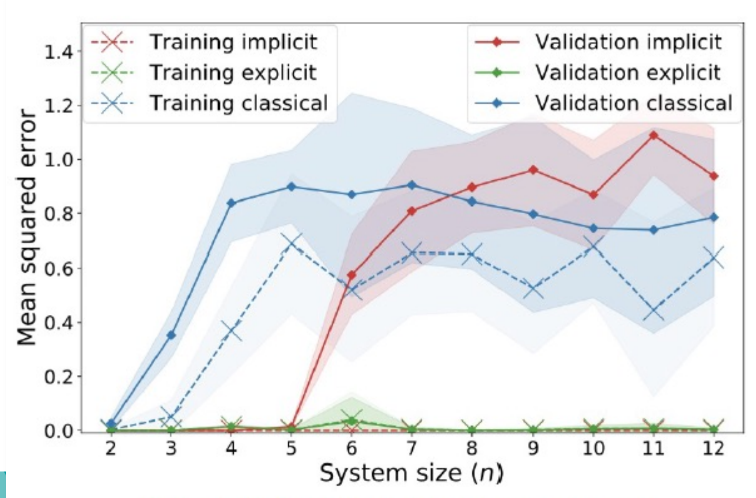
**Ex:**

- 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



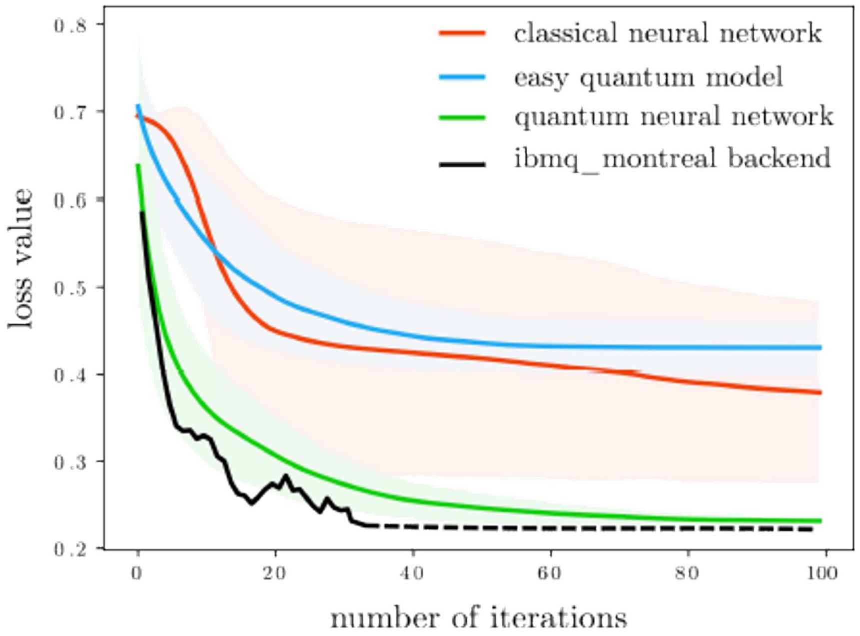




PCA on 28x28 fashion-MNIST dataset, ZZ feature encoding + hardware-efficient variational unitary

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

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

# Model Convergence and Barren Plateau

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

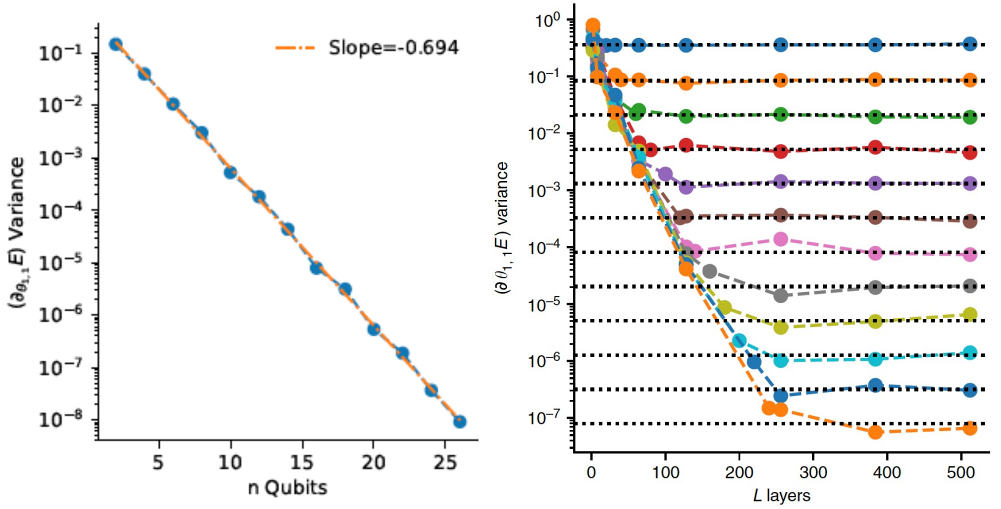
Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)

- Convergence still possible if gradients consistent between batches.

**Quantum gradient decay exponentially in the number of qubits**

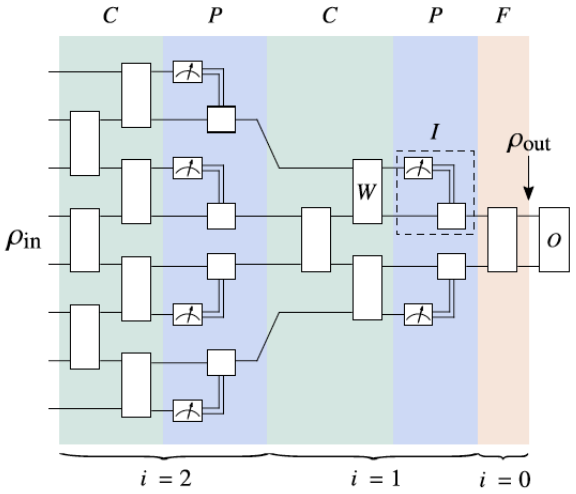
- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.,* arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011. )
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12,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

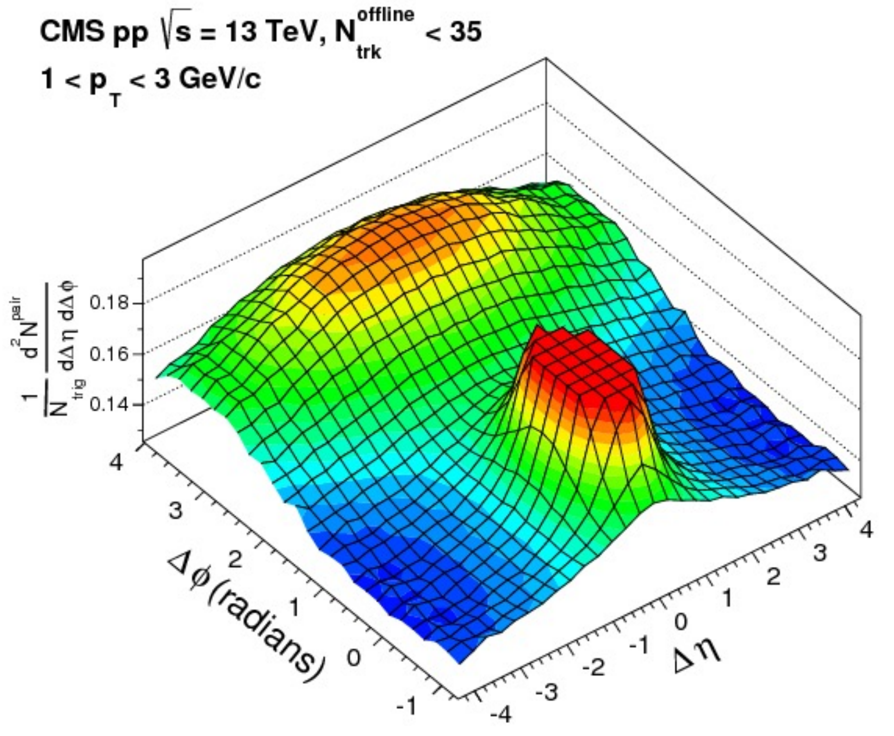


# Practical advantage

**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

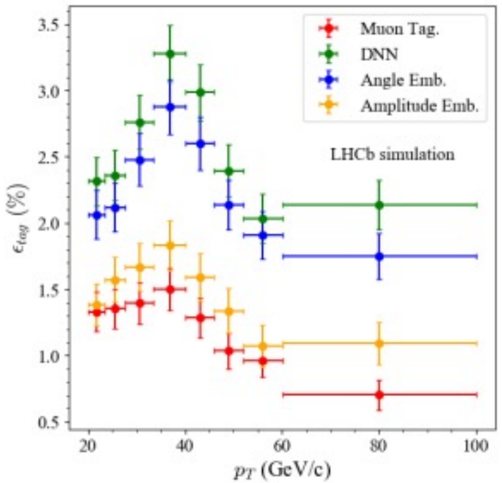
**A change of paradigm could reflect in interesting insights**

- 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).

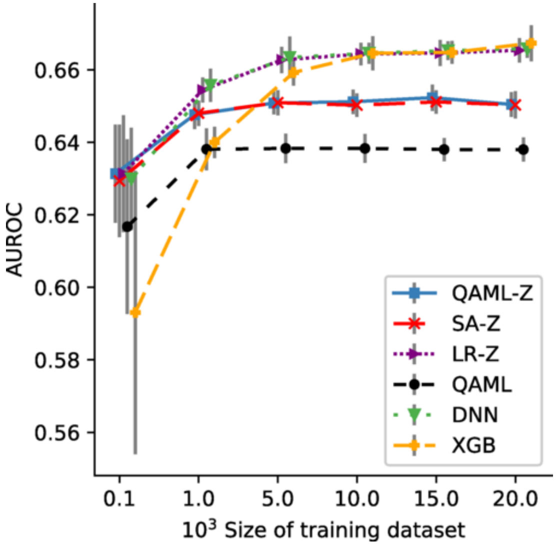
See M. Grossi summary at the 2022 CERN Openlab Technical Workshop : https://indico.cern.ch/event/1100904/contributions/4775169/

# QML in High Energy Physics

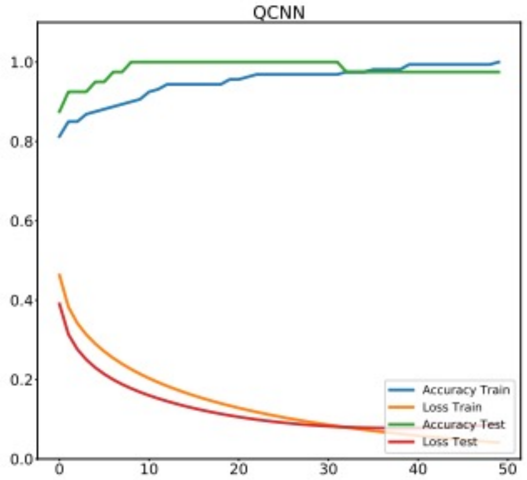



Alessio Gianelle, Patrick Koppenburg, Donatella Lucchesi, Davide Nicotra, Eduardo Rodrigues, Lorenzo Sestini, Jacco de Vries, and Davide Zuliani. **Quantum Machine Learning for *b*-jet identification.** arXiv:2202.13943, 2022.

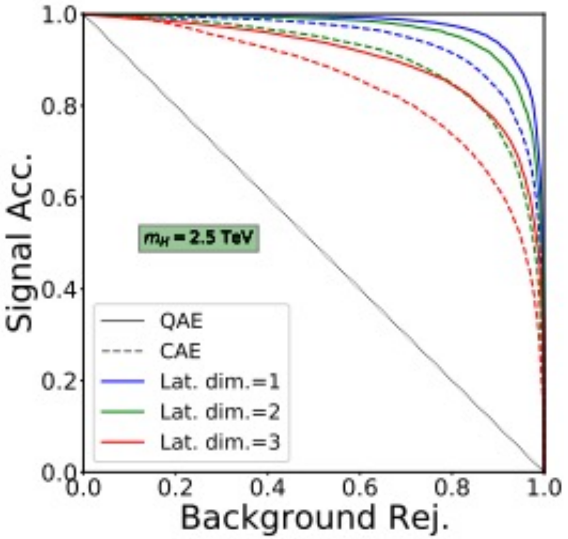
Alexander Zlokapa, Alex Mott, Joshua Job, Jean-Roch Vlimant, Daniel Lidar, and Maria Spiropulu. **Quantum adiabatic machine learning by zooming into a region of the energy surface.** Physical Review A, 102:062405, 2020. DOI:10.1103/PhysRevA.102.062405.



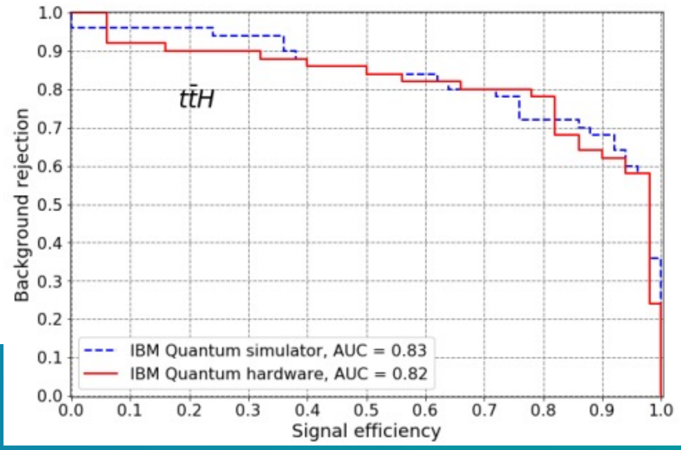

Samuel Yen-Chi Chen, Tzu-Chieh Wei, Chao Zhang, Haiwang Yu, and Shinjae Yoo. **Quantum convolutional neural networks for high energy physics data analysis.** arXiv preprint: 2012.12177, 2020.



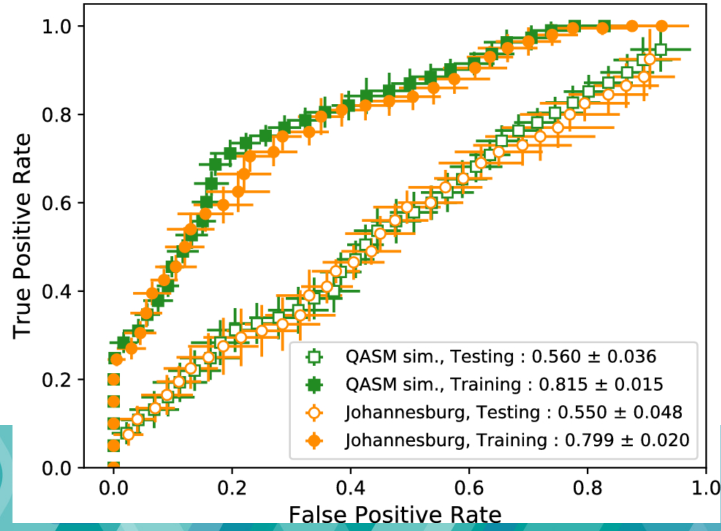

Vishal S Ngairangbam, Michael Spannowsky, and Michihisa Takeuchi. **Anomaly detection in high-energy physics using a quantum autoencoder**. arXiv preprint arXiv:2112.04958, 2021.




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

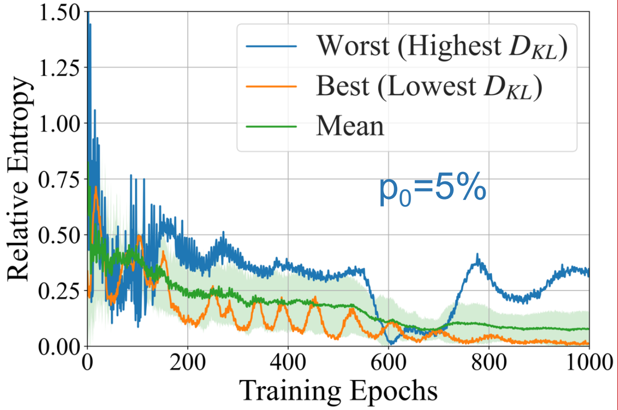



Koji Terashi, Michiru Kaneda, Tomoe Kishimoto, Masahiko Saito, Ryu Sawada, and Junichi Tanaka. **Event classification with quantum machine learning in 20 high-energy physics**. Computing and Software for Big Science, 5(1), January 2021.

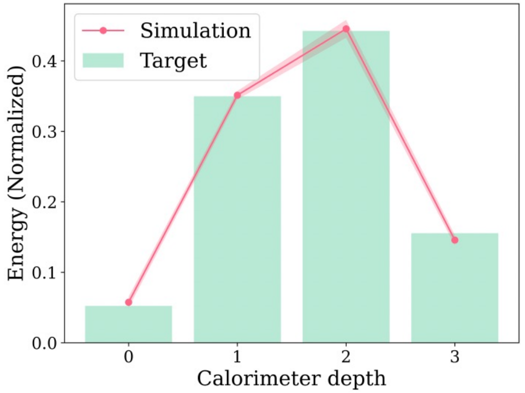


# QML at CERN

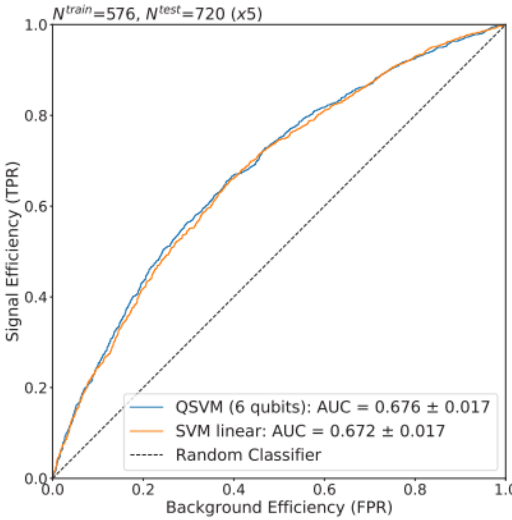
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." *arXiv preprint arXiv:2203.01007* (2022).



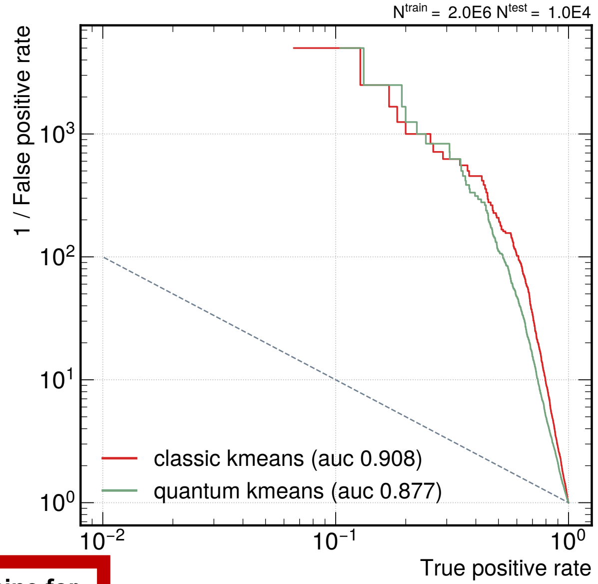

Chang S.Y. *et al.,* **Running the Dual-PQC GAN on Noisy Simulators and Real Quantum Hardware**, QTML2021, ACAT21



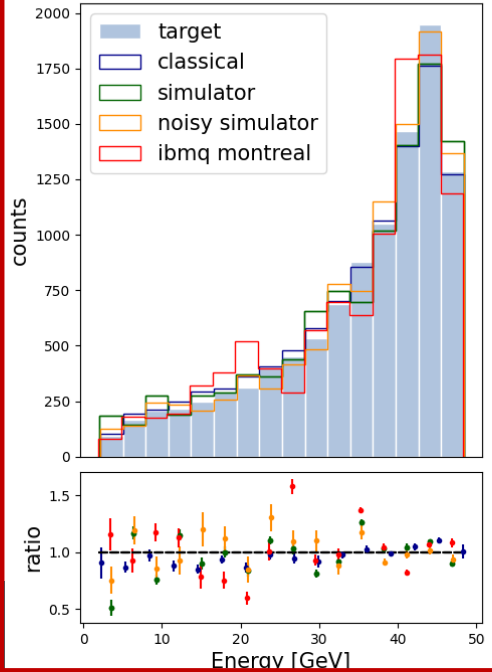

Vasilis Belis, Samuel González-Castillo, Christina Reissel, Sofia Vallecorsa, Elías F. Combarro, Günther Dissertori, and Florentin Reiter. **Higgs analysis with quantum classifi**ers. EPJ Web of Conferences, 251:03070, 2021



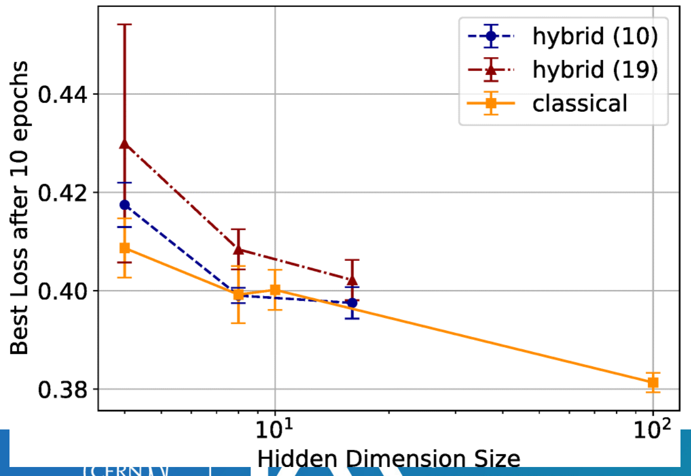

Kinga Wozniak, **Unsupervised clsutering for a Randall–Sundrum Graviton at 3.5TeV narrow resonance**



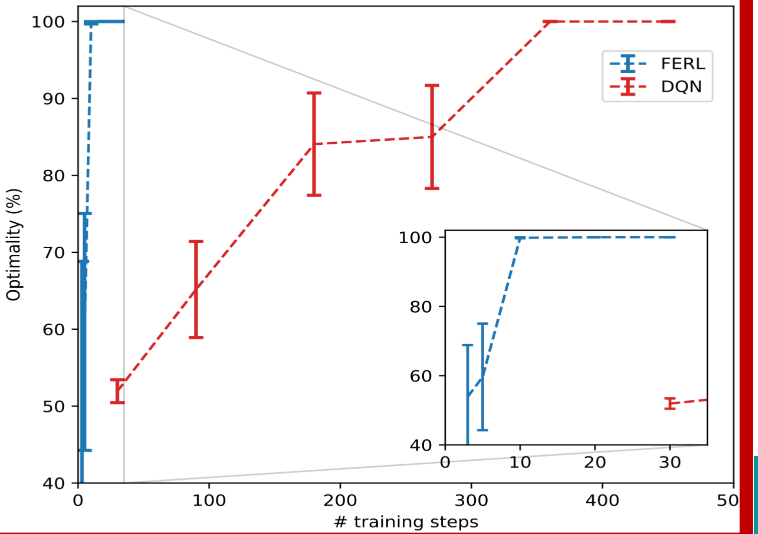

O. Kiss, **Quantum Born Machine for event generation**, ACAT2021



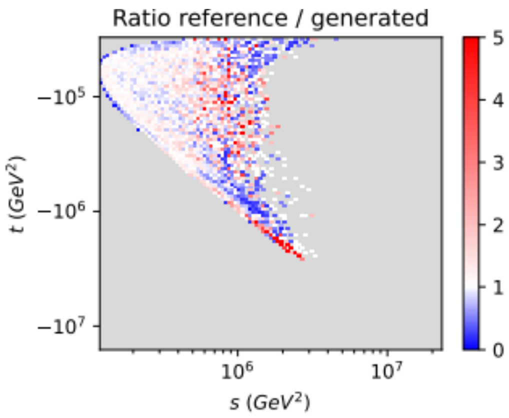

Tüysüz, Cenk, et al. "**Hybrid quantum classical graph neural networks for particle track reconstruction**." *Quantum Machine Intelligence* 3.2 (2021): 1-20.




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




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

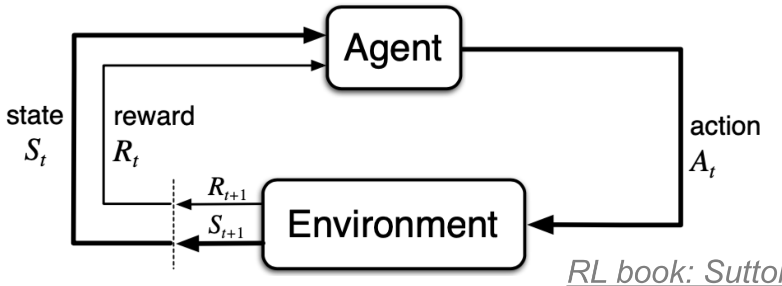


M. Shenk, V. Kain
BQiT 2021
2022 CERN openlab Tech Workshop

# Quantum Reinforcement Learning

**Return** is estimated by **value function *Q(s, a)***

- **Use greedy policy (**maximize *Q(s,a))*
- **Q-learning** – learn Q(s, a) using **function approximator**
  - **DQN: Deep Q-learning** *(feed-forward neural network)*
  - **QBM-RL** *(Quantum Boltzmann Machine)*

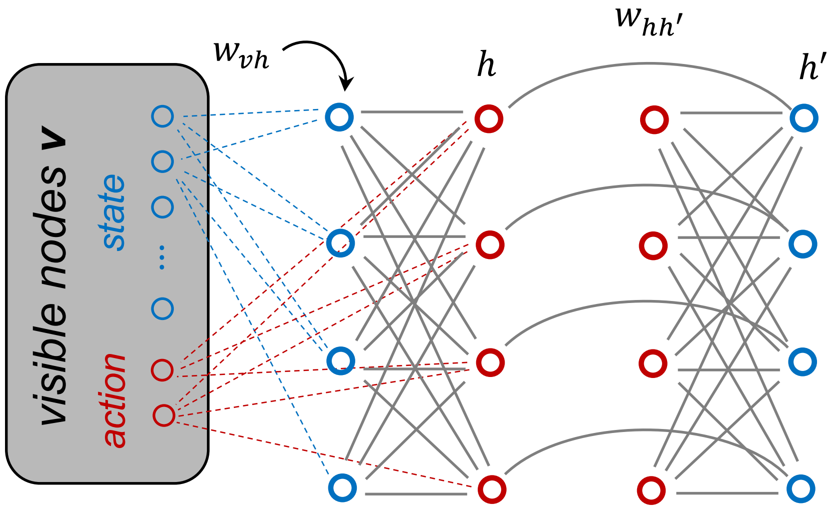



RL book: Sutton & Barto

**Free Energy RL: clamped QBM**

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

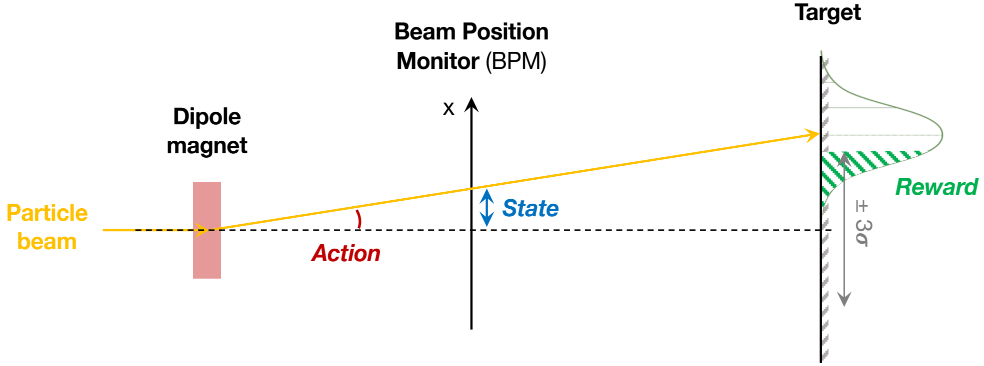
**Clamped QBM**




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

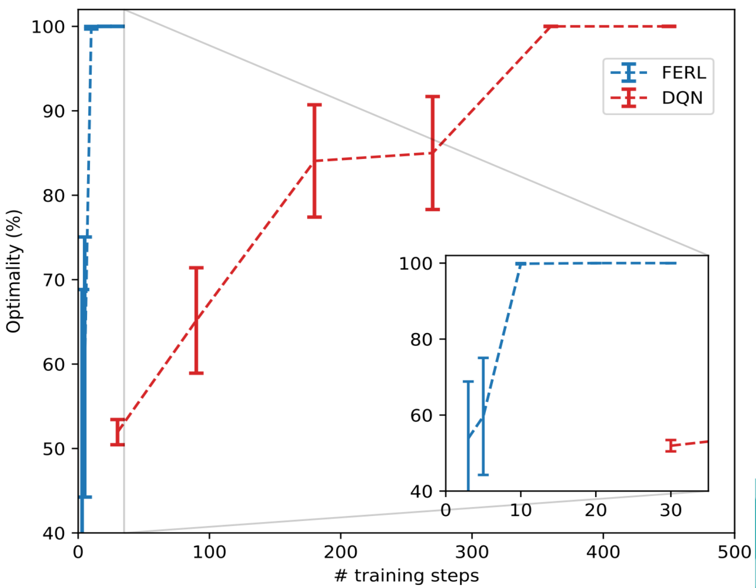
# Beam optimisation in linear accelerator

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

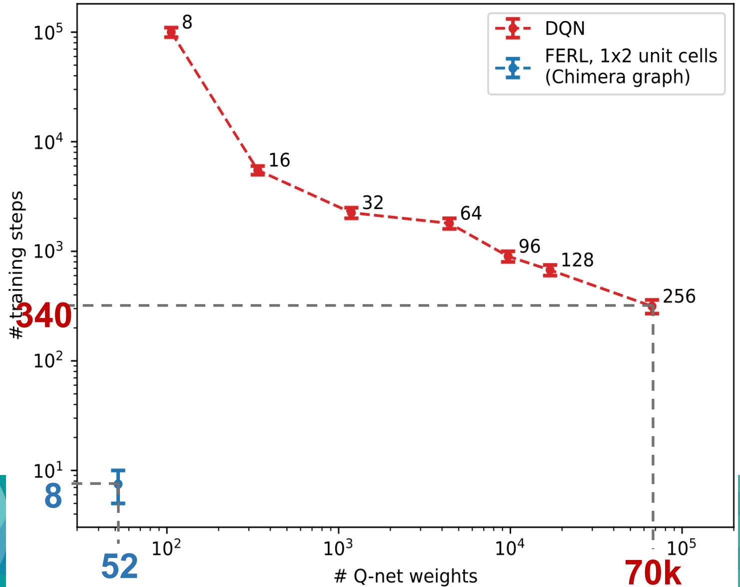



- **Training efficiency:** FERL **massively** outperforms classical Q-learning *(8±2 vs. 320±40 steps)*
- **Descriptive power:** QBM can reach high performance with **much fewer weights** than DQN *(52 vs. ~70k)*

**Training efficiency**



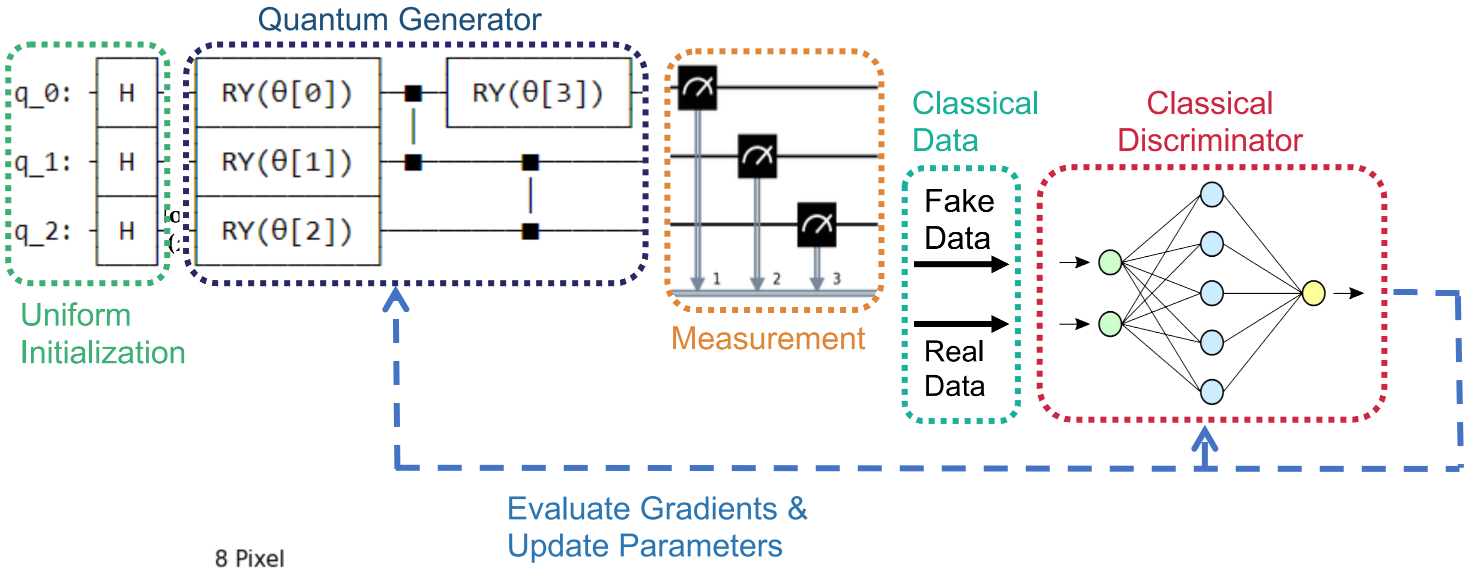

**Training efficiency vs. # Q-net / QBM weights**

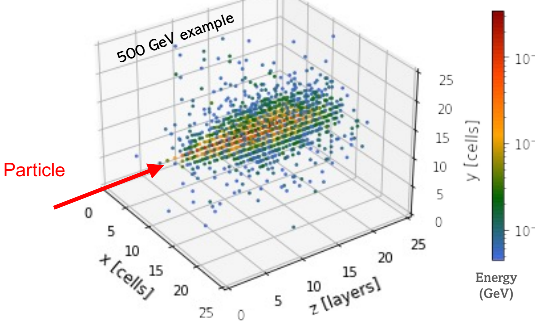


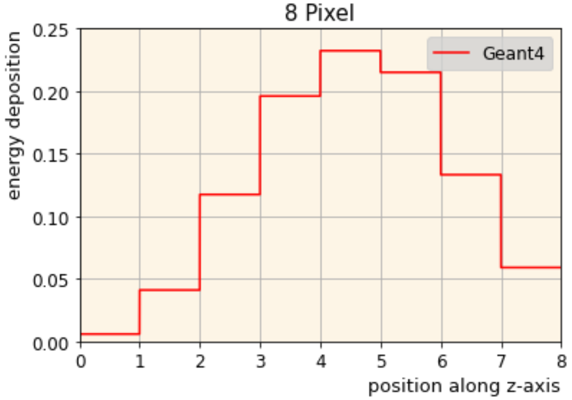
# Quantum Generative Adversarial Networks

## *Generating Energy Profiles in HEP 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).

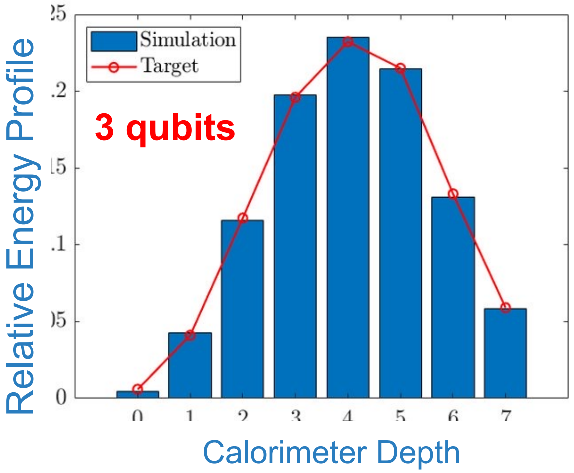
# Quantum generation of energy profiles

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

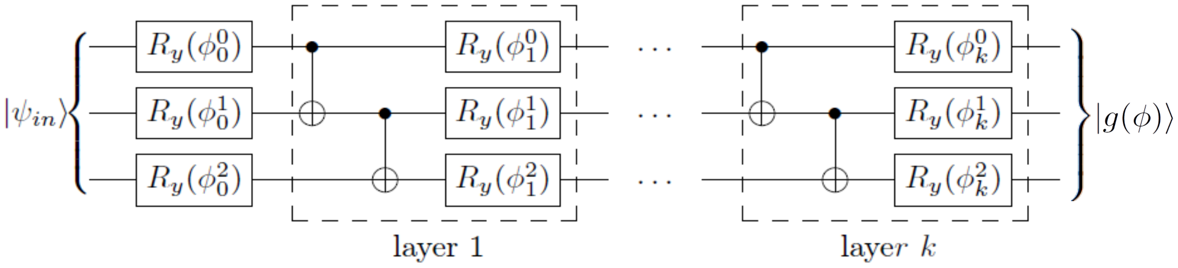
**Simplify simulation problem**

1D & 2D energy profiles from detector

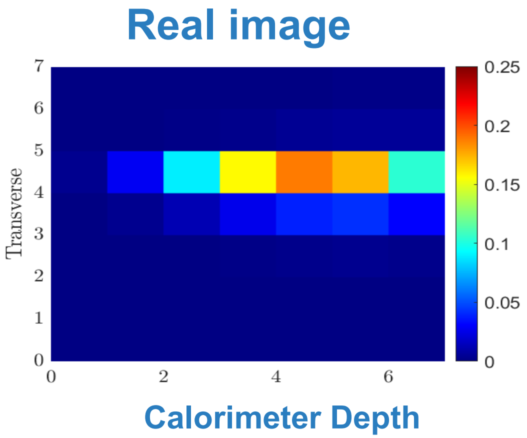
Train a **hybrid classical-quantum** GAN to generate **average image**

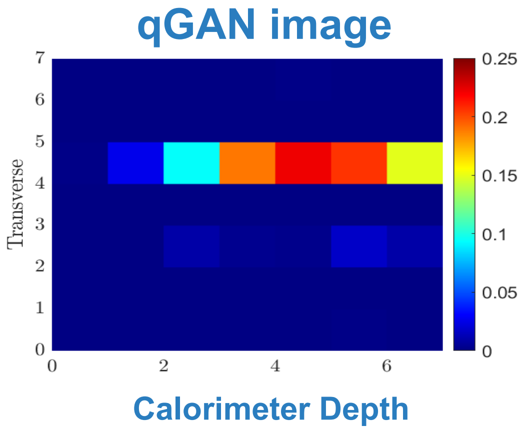



### Quantum Generator: 3 $R_y$ layers




6 qubits



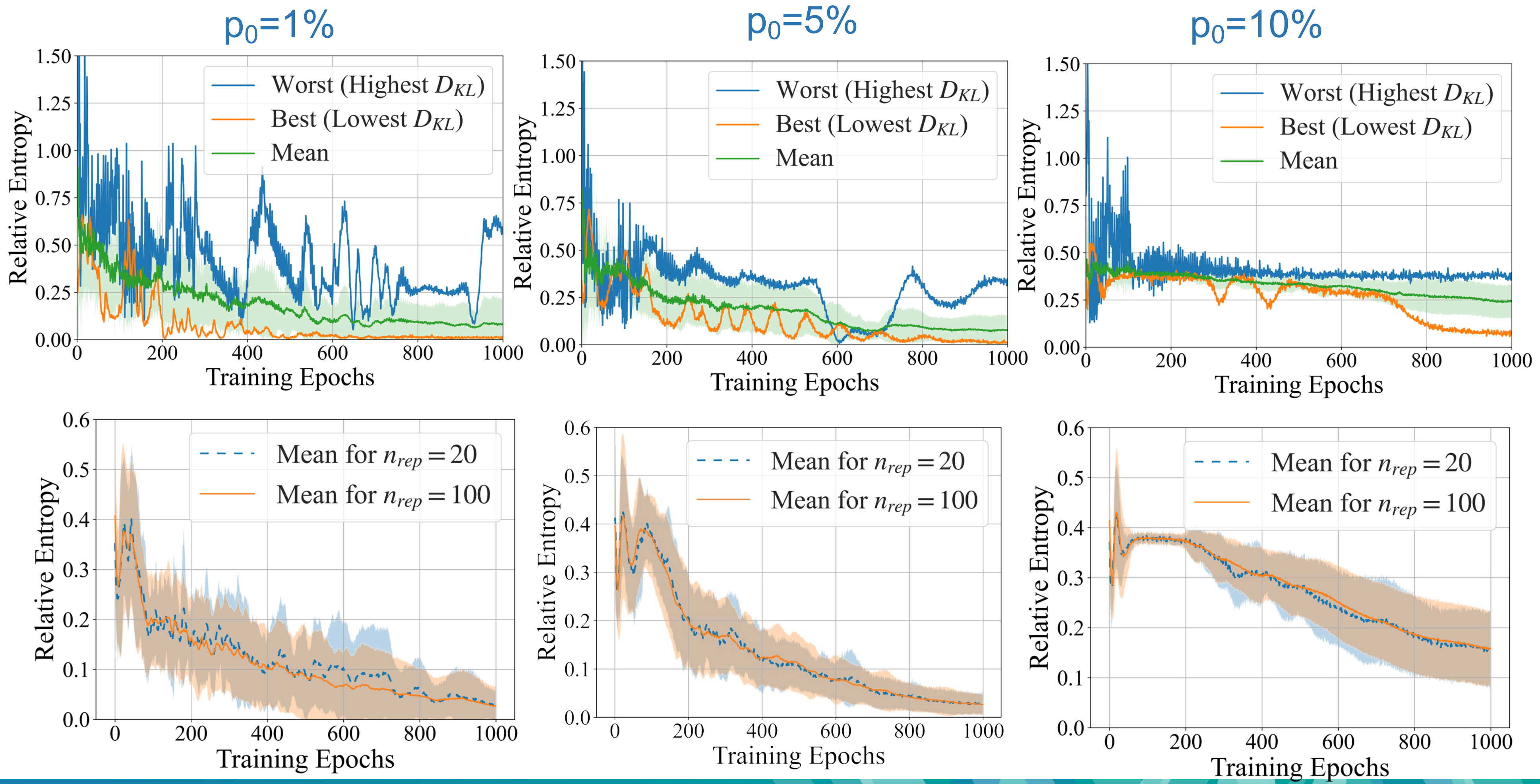




1 Zoufal, C., Lucchi, A. & Woerner, S. Quantum Generative Adversarial Networks for learning and loading random distributions. *npj Quantum Inf* **5,** 103 (2019). https://doi.org/10.1038/s41534-019-0223-2

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

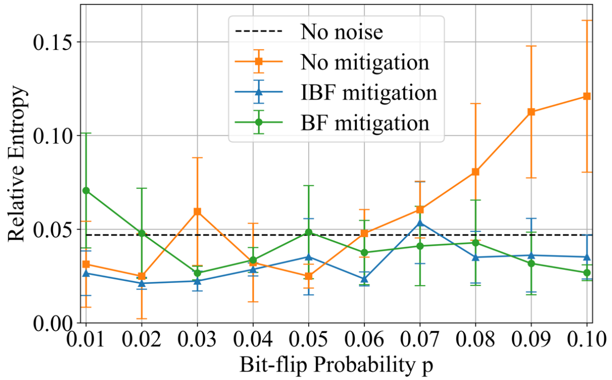


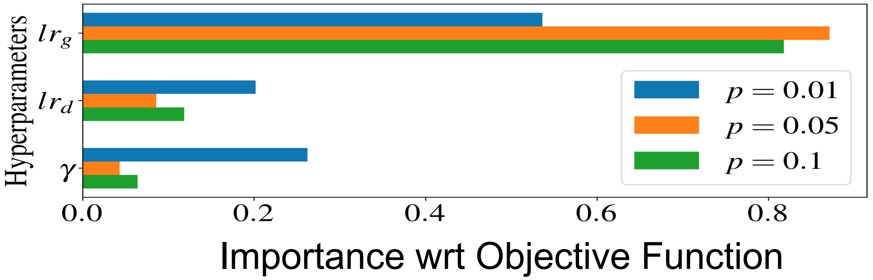
# Running the model on noisy devices

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

Train on noisy simulator

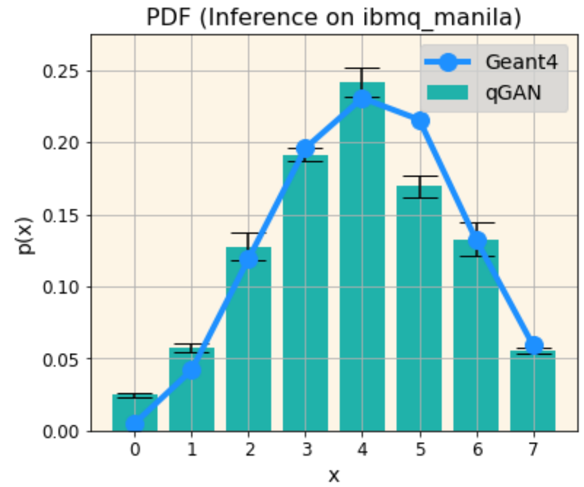
- Evaluate importance of training hyperparameters
- **Error mitigation needed only** for **higher** noise level

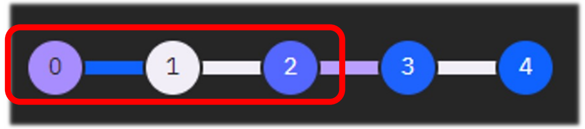



Inference on IBM Q Manila hardware

- Maintain good physics perfomance




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


# Thanks!

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