QUANTUM TECHNOLOGY INITIATIVE

CERN Main Auditorium

QUANTUM TECHNOLOGY CONFERENCE

QT4HEP

1 - 4 November, 2022

CERN QTI
Algorithm overview

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CERN IT Innovation

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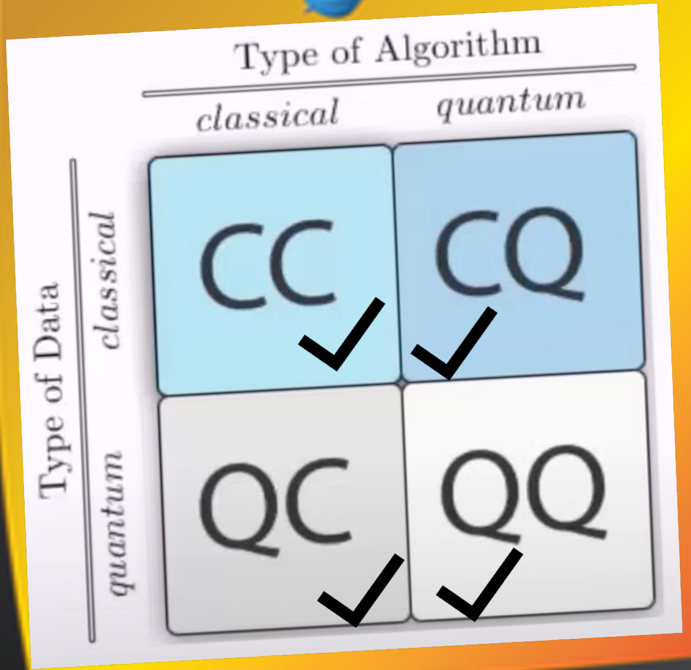
Computing & Algorithms

Assess the areas of potential quantum advantage in HEP - classification, anomaly detection, clustering, generative model

Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

Develop common libraries of algorithms methods, tools - benchmark classical frameworks and automatize procedure on Hardware

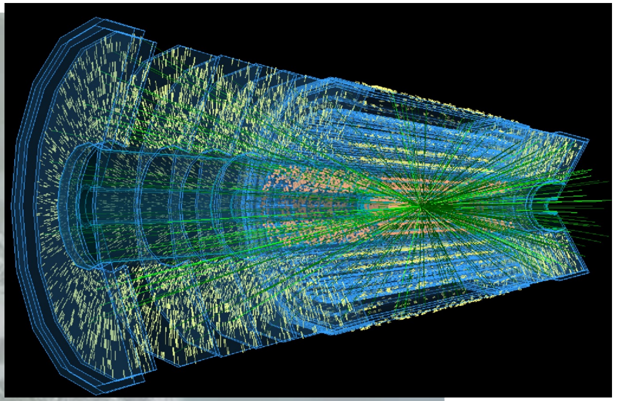


$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c. + \Psi_i y_{ij}\Psi_j\Phi + h.c. + |D_\mu\Phi|^2 - V(\Phi)$$

2013

Theory

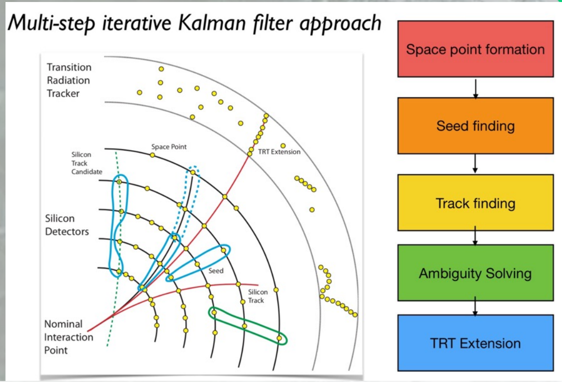
CERN

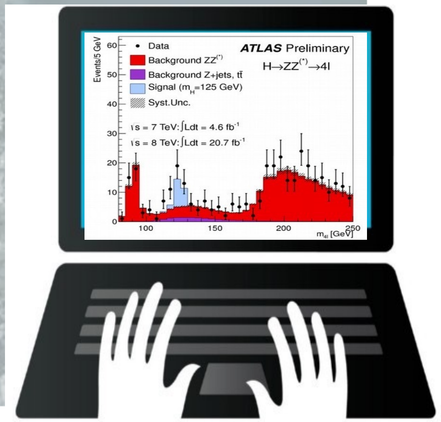


Simulation

Data Acquisition

Data Analysis





QML models implementations for NISQ

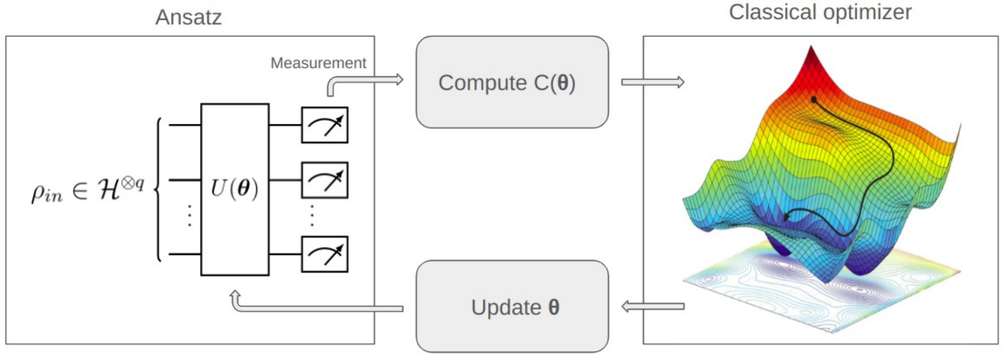
Variational algorithms - EXPLICIT

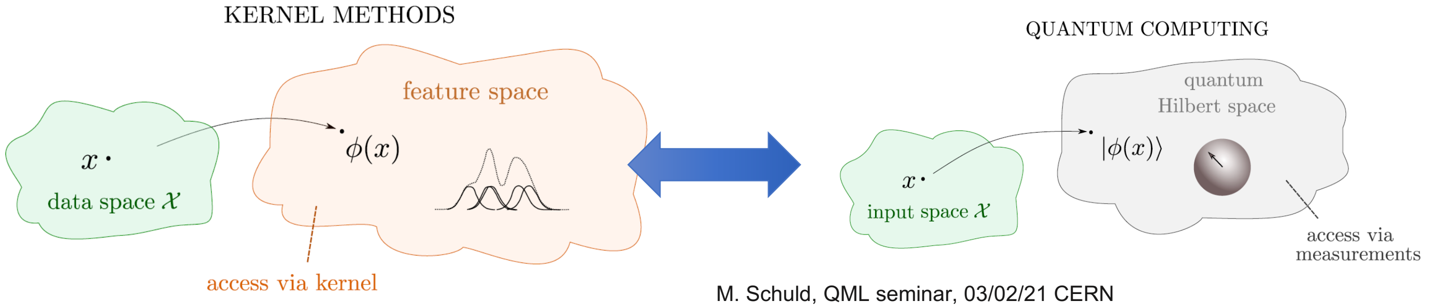
- Flexible parametric ansatz: design can leverage data symmetries[1]
- Can use **gradient-free** methods or **stochastic gradient-descent**
- **Data Embedding** can be **learned**
- **Better generalization**[1]

Kernel methods - IMPLICIT

- **Feature maps** as **quantum kernels**
- **Convex** losses, **global** minimum
- Identify kernel classes that relate to specific **data structures**[3]
- **Better accuracy**[2]

→ What is easiest to use/define?





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

1-Bogatskiy, Alexander, et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020

2-S.Jerbi at all., Quantum Machine Learning Beyond Kernel Methods https://arxiv.org/abs/2110.13162

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

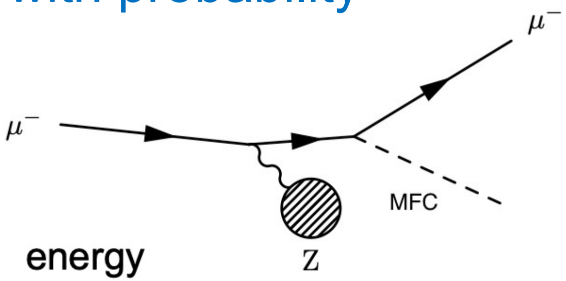
Do they really differ? Where to focus?

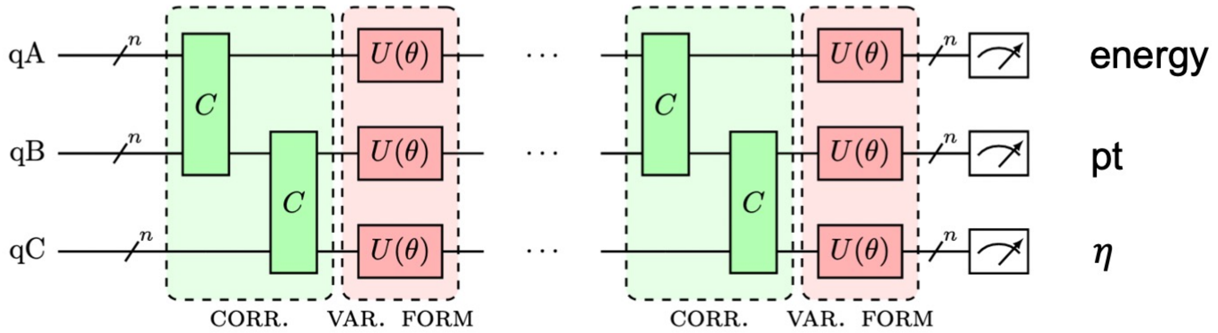
Quantum Circuit Born Machine for event generation

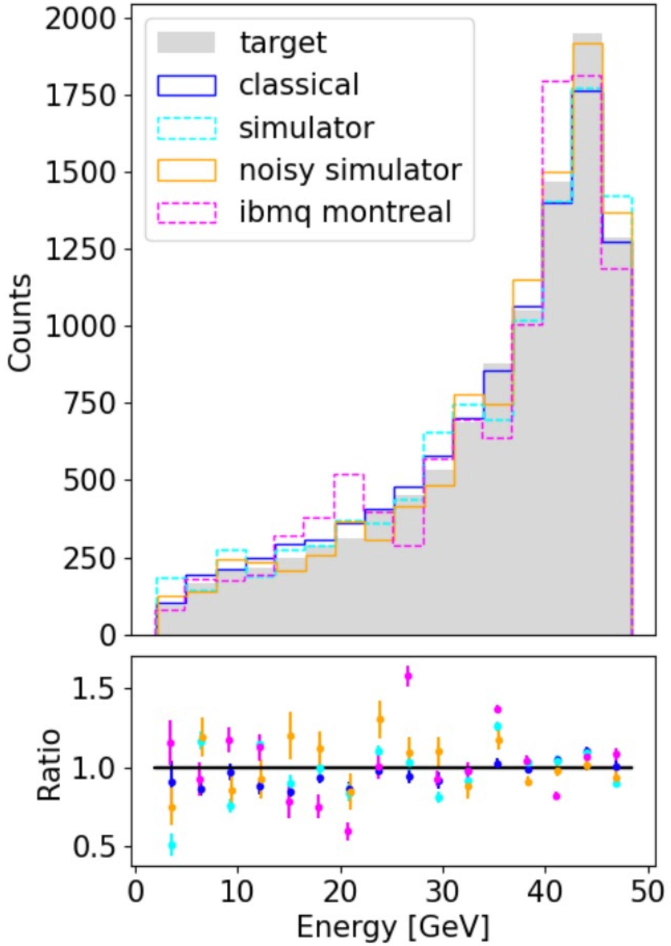
Kiss O., Grossi M. et all., **Conditional Born machine for Monte Carlo events generation**, *Phys. Rev. A* ***106****, 022612 (2022)*

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

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







- Generate **discrete PDFs** (continuous in the limit #qubits $\to \infty$)
- 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

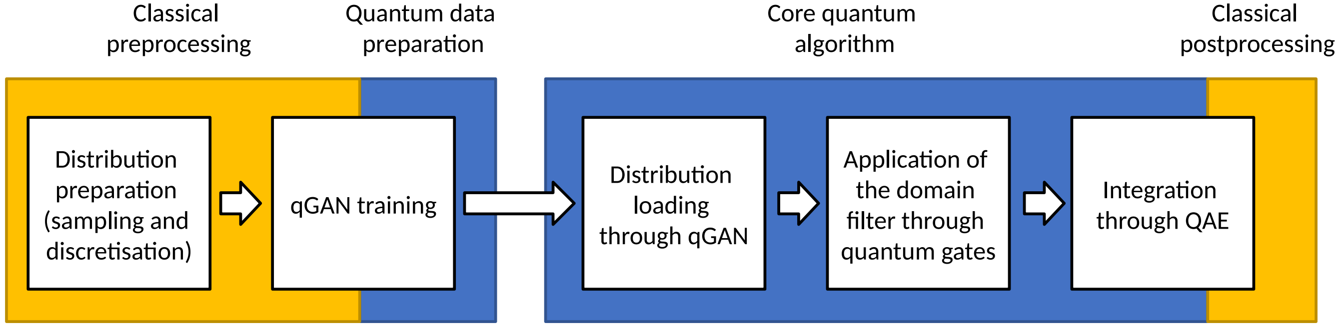
- **Pros**: relativly easy to optimize, **Cons**: empircally less efficient than an adversarial approach

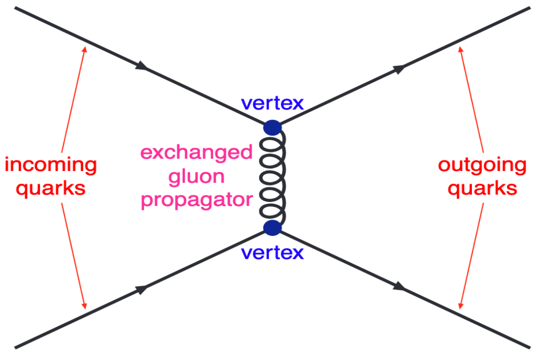
Coyle, B., Mills, D. et al, **The Born supremacy.** In: *npj Quantum Inf 6, 60* (2020)

Agliardi, Grossi, et al. "**Quantum integration of elementary particle processes**." https://doi.org/10.1016/j.physletb.2022.137228

Cross section integration

- **Cross section integration** using **Quantum Amplitude Estimation**
- **Focus on electroweak process**





phase-space factor

$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

matrix element

phase-space cuts

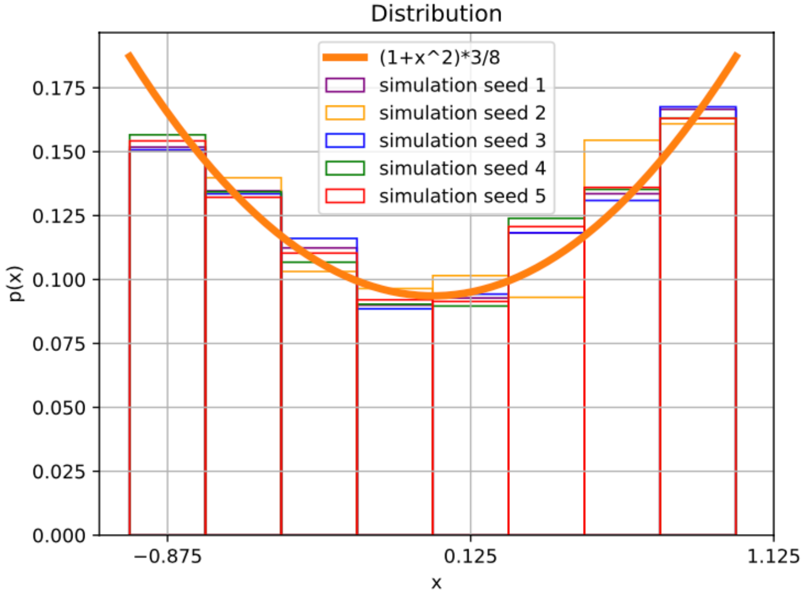
- Data encoding in quantum states affects quality of integration
- Test **QGAN for data embedding** and compare to direct loading

Test on $1 + x^2$ distribution:

- 10k events, 3 qubits, circular entanglement

$$G(\phi)\,|\psi_{in}\rangle = |g(\phi)\rangle = \sum_{i=0}^{N-1} \sqrt{p_g^i(\phi)}\,|i\rangle$$

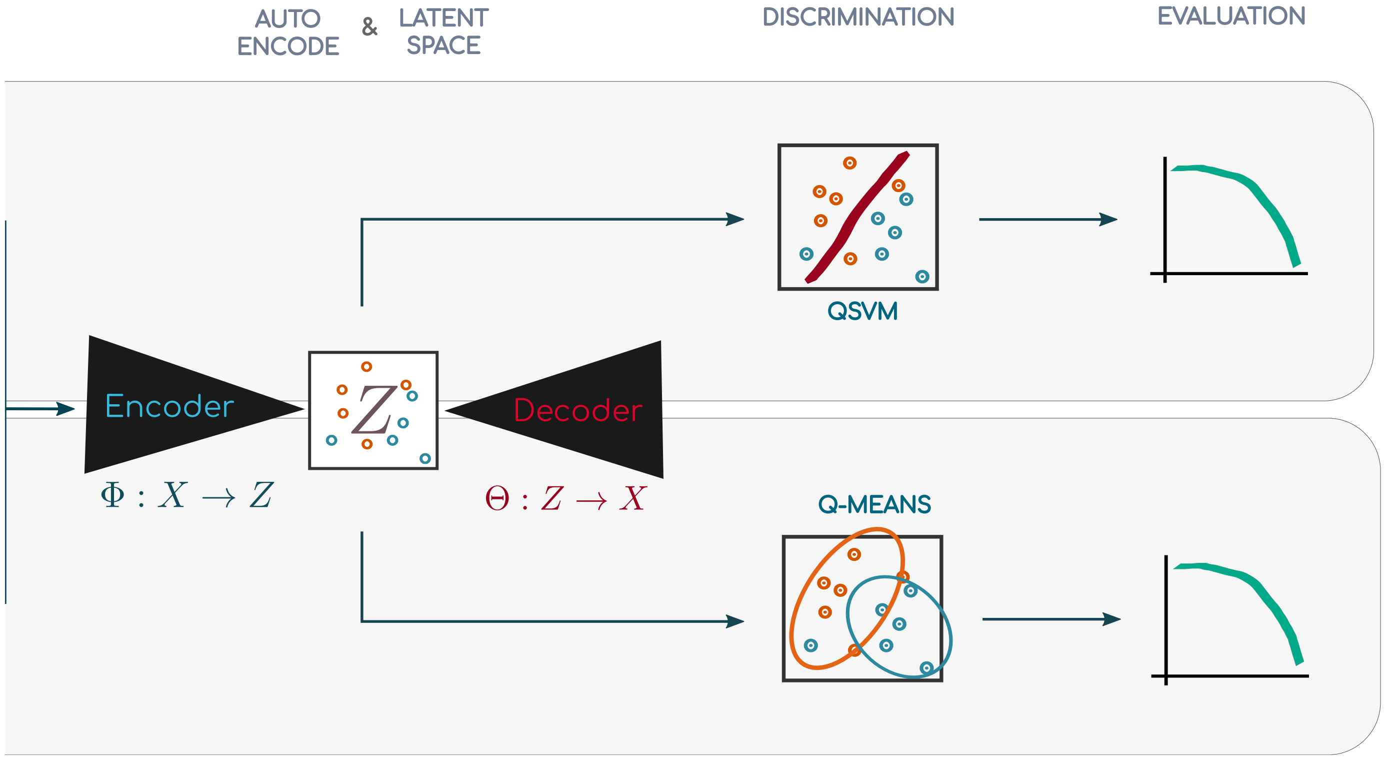
Loading	Difference per bin [%] Min.	Max.	Average	σ_x
Direct	+0.207	−1.88	1.35	1.80×10^{-3}
qGAN default	+2.36	−21.1	8.51	0.0118
qGAN optimised	−0.995	−12.4	4.65	7.00×10^{-3}



Quantum Anomaly Detection in the latent space

- Models:

  - Unsupervised *kernel machine*,
  - *Q-means, Q-medians* (clustering algorithms)



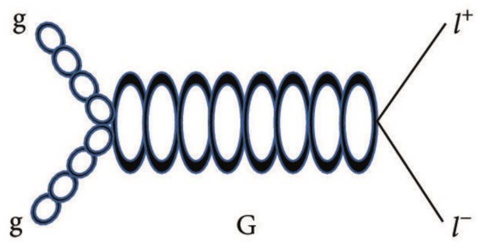
- Data:

  - Anomaly *signatures*:

    Narrow and Broad Graviton resonance G → W^+W^-

    New boson A → HZ → ZZZZ

  - SM *background* constitutes of QCD dijet events: m_{JJ} resonance spectrum
  - Dimensionality reduction: *Convolutional AE*



Quantum Anomaly Detection in the latent space

Approach and Results

Study the performance as a function of:

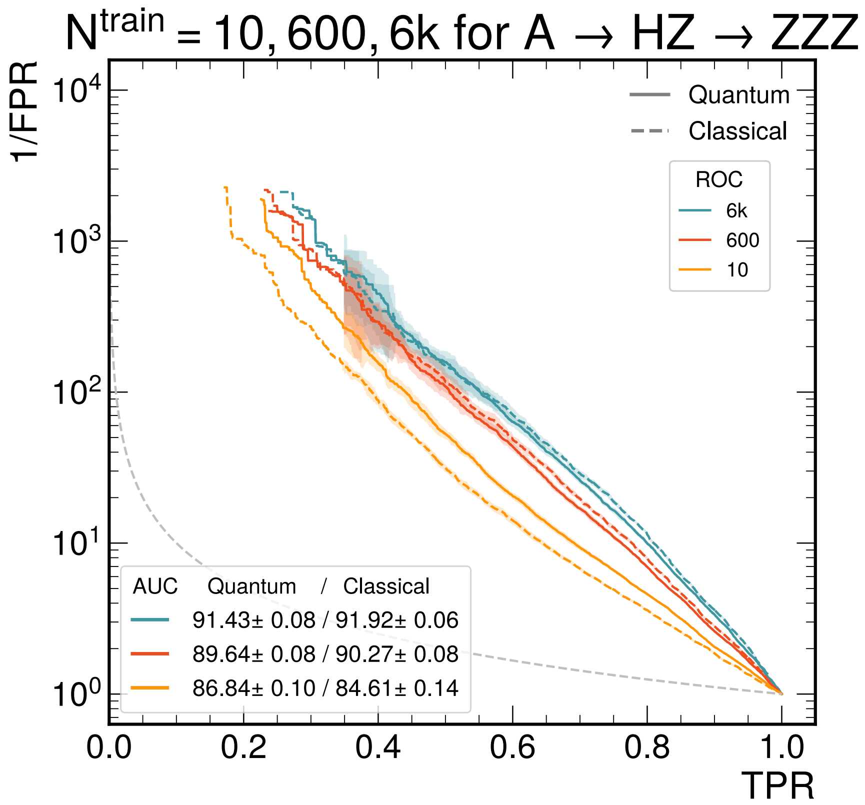
- N_{train}
- Dimensionality of the data feature
- *Expressibility* and *entanglement capability* of data encoding feature map
- Clustering:

  - Quantum distance calculation

  - Classic minimization to the closest cluster

  - Cluster median calculation

  (Quantum distance + heuristics)



Q-medians clustering

A priori methodology to assess Quantum Advantage (QA)

From complexity-theoretical argument it can be proved a rigorous prediction error upper bound which defines the metrics defined in [1], implemented in [2]

$$\mathbb{E}_{\mathbf{x}}|h(\mathbf{x}) - y(\mathbf{x})| \leq \mathcal{O}\left(\sqrt{\frac{s_{K,\lambda}(N)}{N}}\right)$$

- Geometric Difference – g_{CQ} (λ)
- Approximate Dimension – d
- Model Complexity – $s_{K,\lambda}$ (N)

geometry test

- $g_{CQ} \ll \sqrt{N}$
  - ***dimensionality test***
    - $d \ll N$ → ***Classical*** ✓
    - ***else*** → ***Classical Quantum*** ✓/✗
- $g_{CQ} \propto \sqrt{N}$
  - ***complexity test***
    - $s_C \ll N$ → ***Classical*** ✓
    - $s_Q \ll N$, $s_C \approx N$ → ***Potential QA***
    - ***else*** → ***Classical Quantum*** ✓/✗

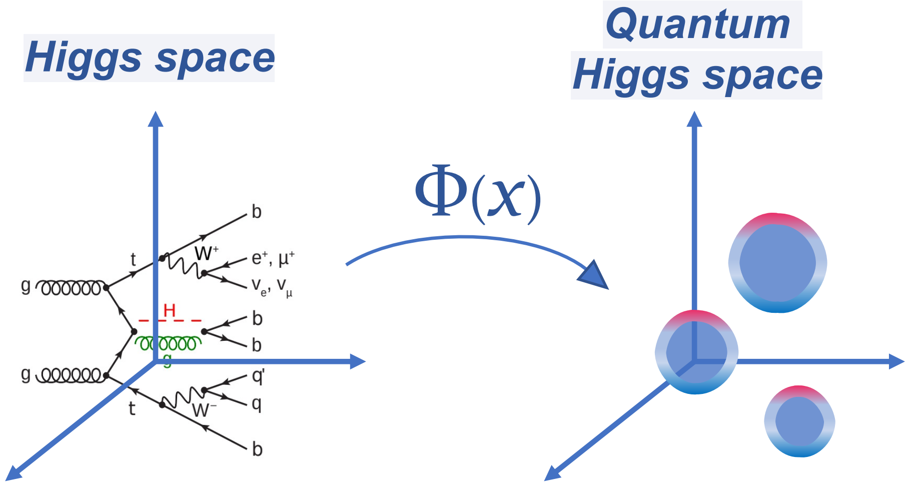
Constraints:

- Encoding (feature) map of classical and quantum kernels
- Data structure - complex distribution function, dimensionality of the input space…
- Optimization of relevant parameters λ, γ

*[1] HY. Huang et al, Nature Communication **12**, 2631 (2021)*
[2] F.Di Marcantonio et all., QuASK -- arXiv:2206.15284

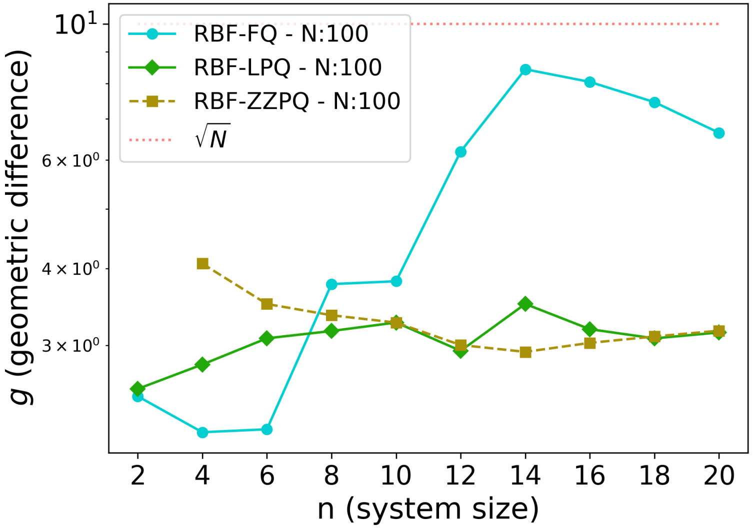
Interpretation in HEP

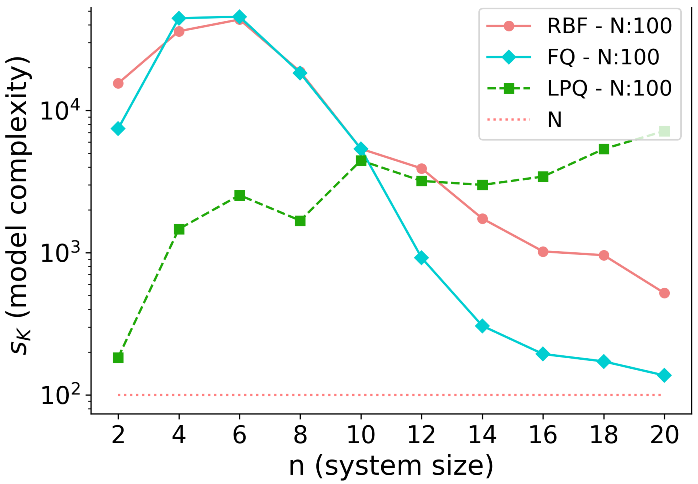
- From general observation:
  - ➢ High number of qubits → High expressivity: data lost in the Hilbert space
  - ➢ $d \approx N$ → Low generalization power

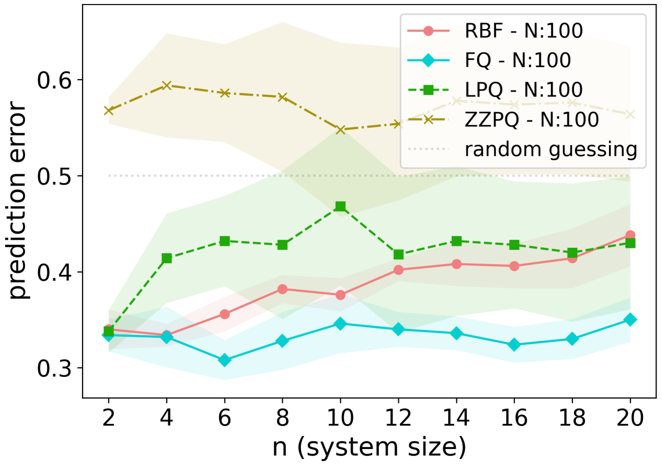


- HEP observation:
  - ➢ Quantum kernels have moderate g_{QC} → Worse performance than the classical counterpart, no QA

EXAMPLE: QSVM for the tt →H →(bb) event classification [2]







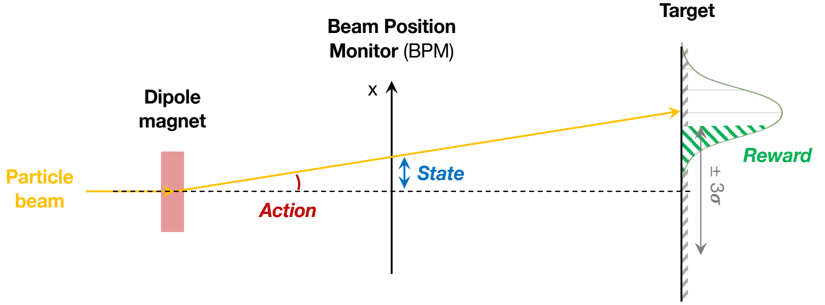
*[2] V. Belis et al, EPJ Web Conf **251**, 03070 (2021)*

Reinforcement Learning for beam steering

Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines – M. Schenk, E.Combarro, M.Grossi et all https://arxiv.org/abs/2209.11044

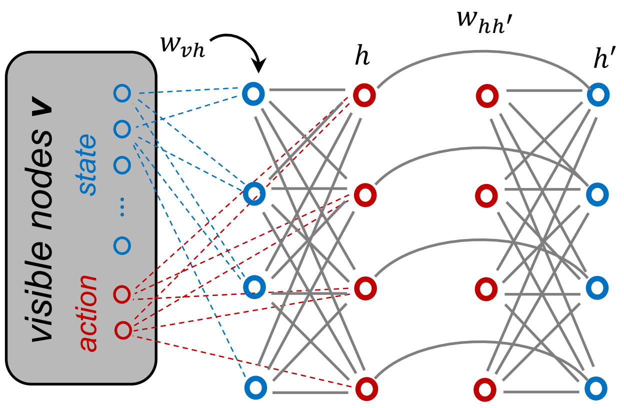
Q-learning – learn value function Q(s, a) using **function approximator**

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

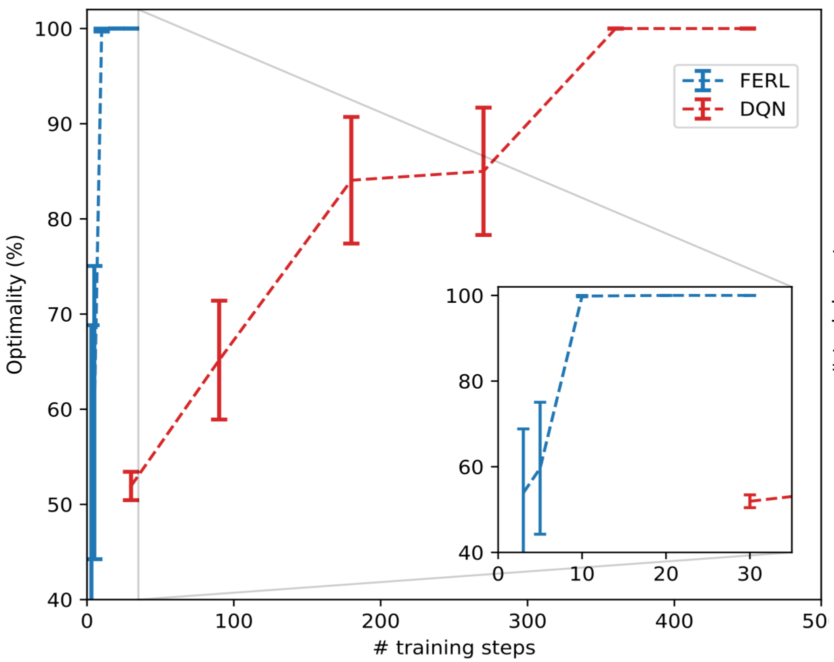


Train QBM on D-Wave 2000q Chimera and 5000q Pegasus

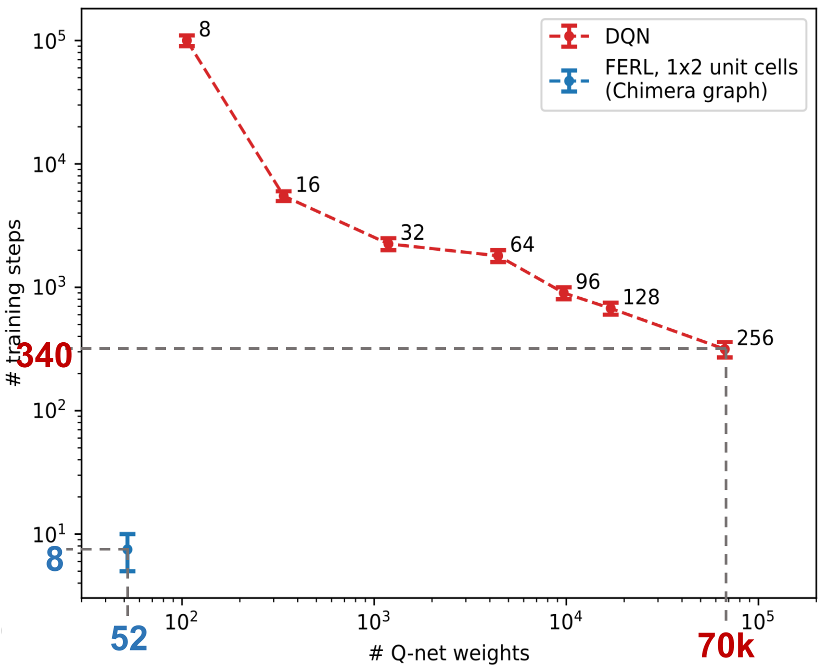
Clamped QBM



Training efficiency

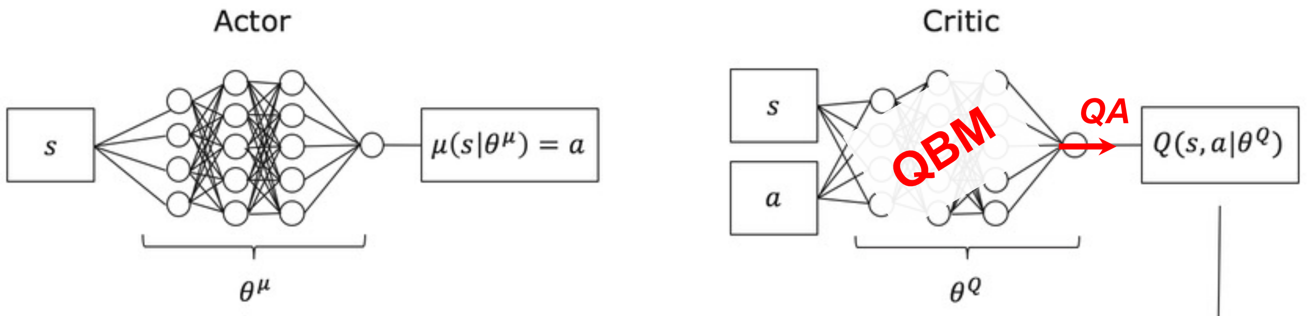


Training efficiency vs. # Q-net / QBM weights

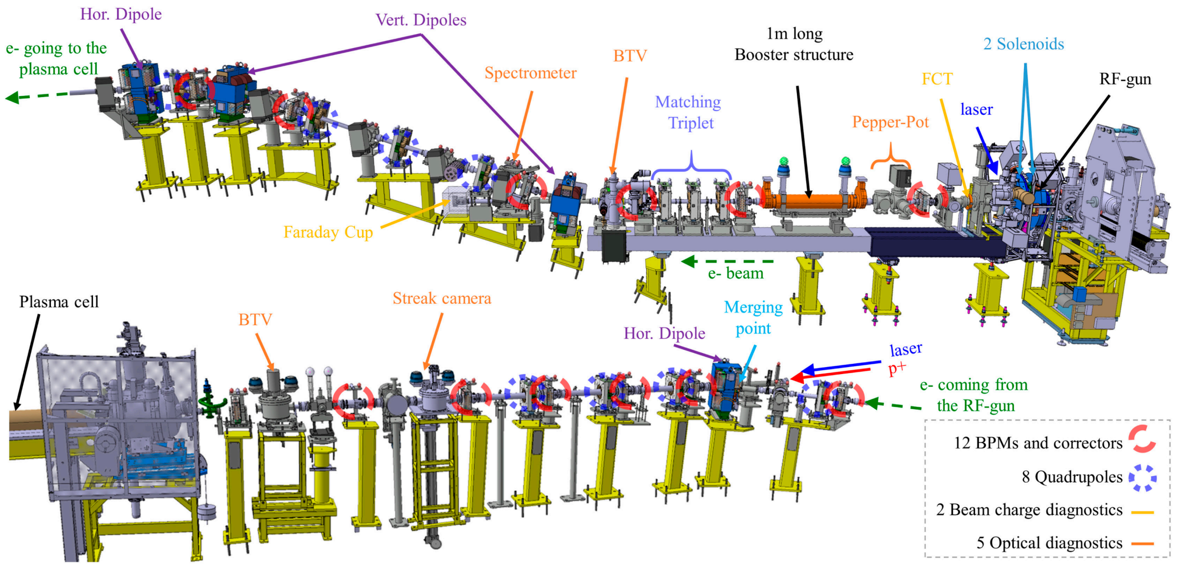


Getting real…

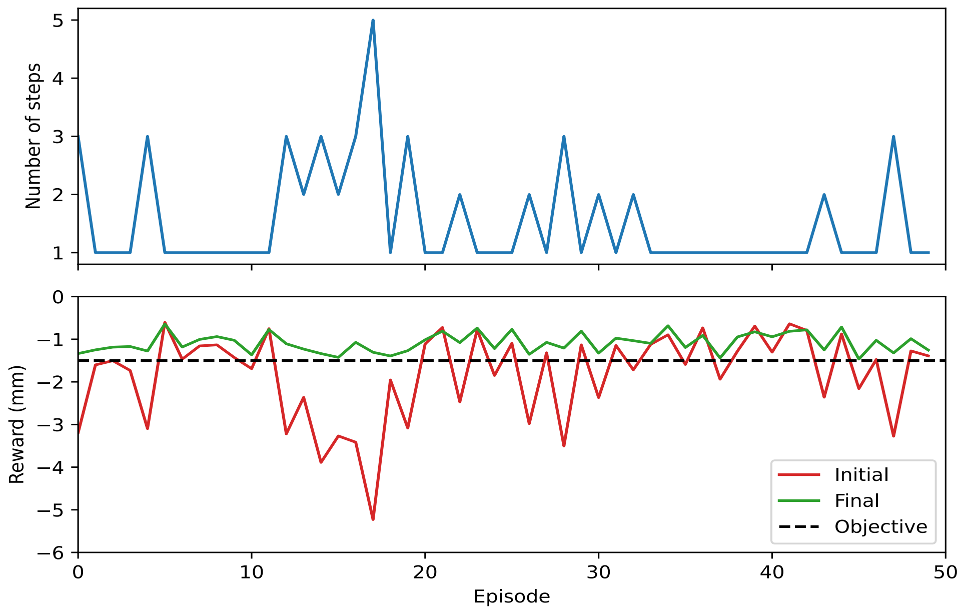
- **AWAKE electron beam line (10BPM)**
  https://gitlab.cern.ch/be-op-ml-optimization/envs/awake



Policy Gradient: $\nabla_{\theta^\mu}\mu = \mathbb{E}_\mu[\nabla_{\theta^\mu}Q(s,\mu(s|\theta^\mu)|\theta^Q)] = \mathbb{E}_\mu[\nabla_a Q(s,a|\theta^Q)\cdot\nabla_{\theta^\mu}\mu(s|\theta^\mu)]$



Evaluation on real beam line



- **Actor-critic Q-learning** training on simulated annealing.
- **Successful evaluation the real beam-line**

Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines – M. Schenk, E.Combarro, M.Grossi et all https://arxiv.org/abs/2209.11044

Quantum Fuzzy Logic

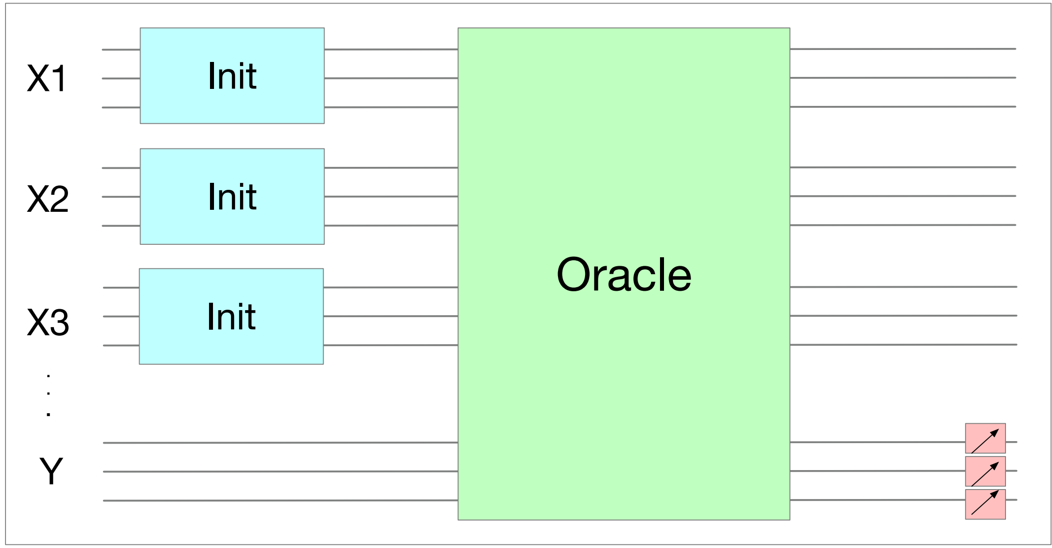
- Fuzzy Logic general applications:
  - ❑ Control systems
  - ❑ Explainable AI inference engines

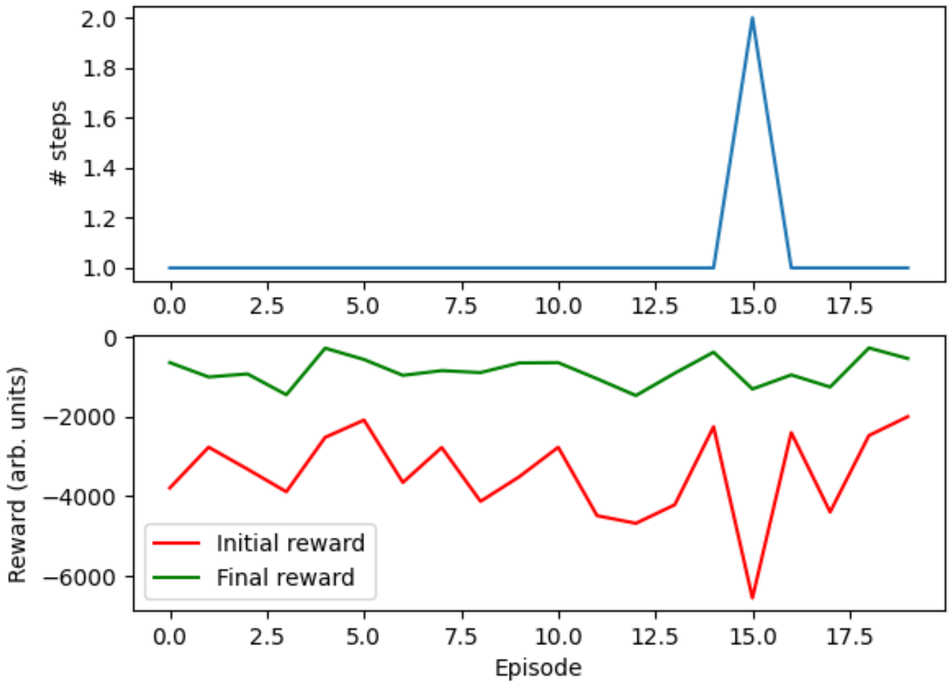
- A *Quantum Fuzzy Inference Engine* (QFIE) has been proposed in [1].

  - ❑ Amplitude encoding of fuzzified values
  - ❑ Formulation of fuzzy rule base as a *quantum oracle*

→ Advantages of a quantum fuzzy inference engine:

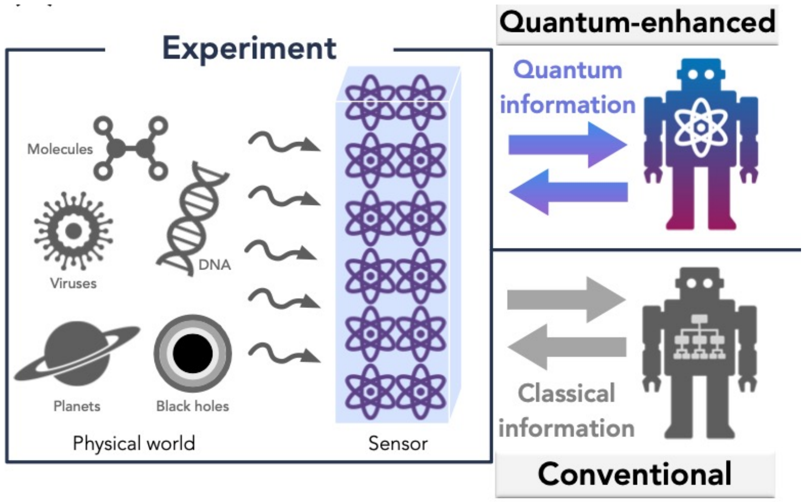
1. Exponential advantage in the number of queries to the oracle
2. Quantum computers can be programmed with linguistic rules.





[1] Acampora, Giovanni, Roberto Schiattarella, and Autilia Vitiello. "On the Implementation of Fuzzy Inference Engines on Quantum Computers." IEEE Transactions on Fuzzy Systems (2022).

Quantum machine learning for quantum data



Huang, *et al., Science* **376**, 6598 (2022)

1. Work directly with quantum states.
2. Bypass any classical processing.

Task: Drawing phase diagrams

1. Supervised classification using a convolutional QNN using the groundstates as input data.
2. Advantageous since quantum states are exponentially hard to save classically.
3. Bottleneck: we need access to classical training labels! Interpolation does not work

Cong, *et al., Nat. Phys.* **15**, 1273–1278 (2019)

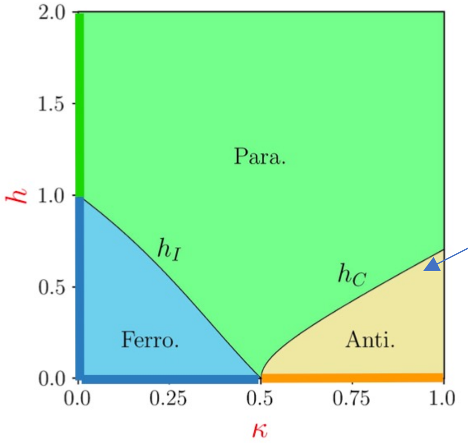
QML for generalization

- **Train in easy (integrable) subregions**
- **Generalize to a full model**
- Model: Axial Next Nearest Neighbor Ising (ANNNI) Hamiltonian:

$$H = J\sum_{i=1}^{N} \sigma_x^i\sigma_x^{i+1} - \kappa\sigma_x^i\sigma_x^{i+2} + h\sigma_z^i,$$

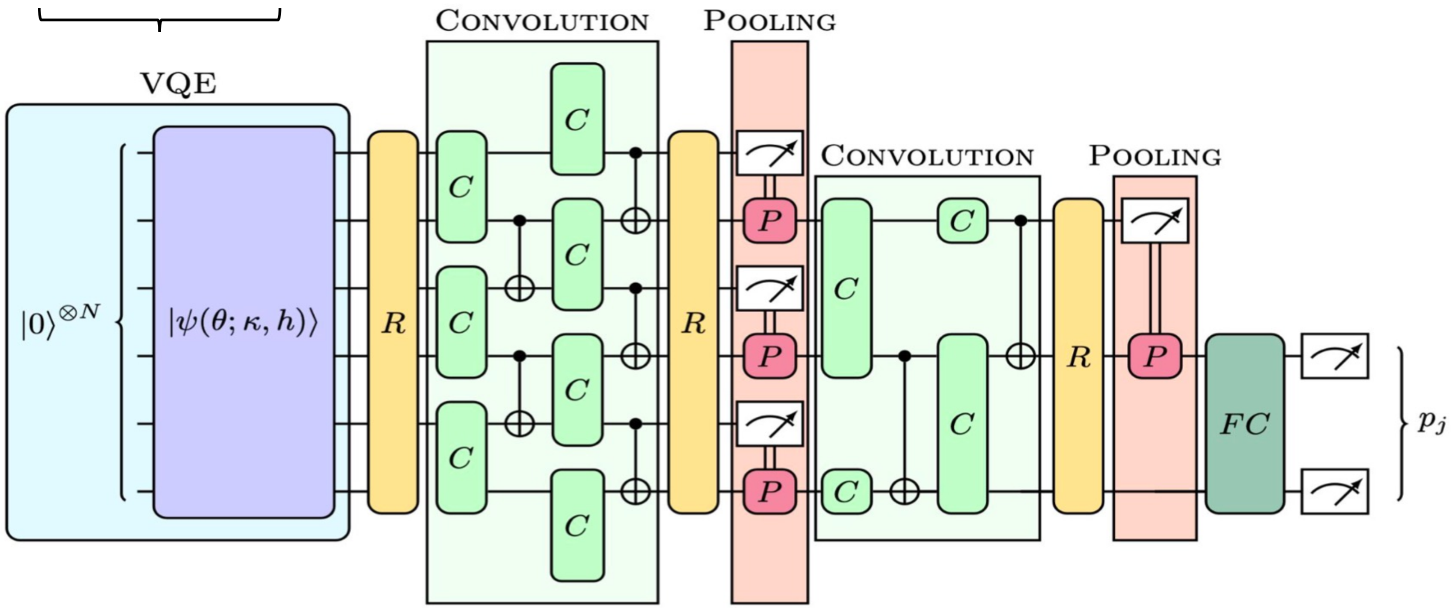
Senk, *Physics Reports*, **170**, 4 (1988)

Which is integrable for $\kappa = 0$ or $h = 0$.



Monte Carlo, DMRG

Variational quantum data



Binary Cross-entropy

Loss: $$\mathcal{L} = -\frac{1}{|\mathcal{S}_X^n|}\sum_{(\kappa,h)\in\mathcal{S}_X^n}\sum_{j=1}^{K} y_j(\kappa,h)\log\left(p_j(\kappa,h)\right)$$

Labels:

- [0,1] ferromagnetic
- [1,0] antiphase
- [1,1] paramagnetic
- [0,0] trash label

Monaco, Kiss, Mandarino, Vallecorsa, Grossi, arXiv: 2208.08748 (2022)

Results

Monaco, Kiss, Mandarino, Vallecorsa, Grossi, arXiv: 2208.08748 (2022)

Learn a similarity function between the data.

Kottman, *et al., Phys. Rev. Research* **3**, 043184 (2021)

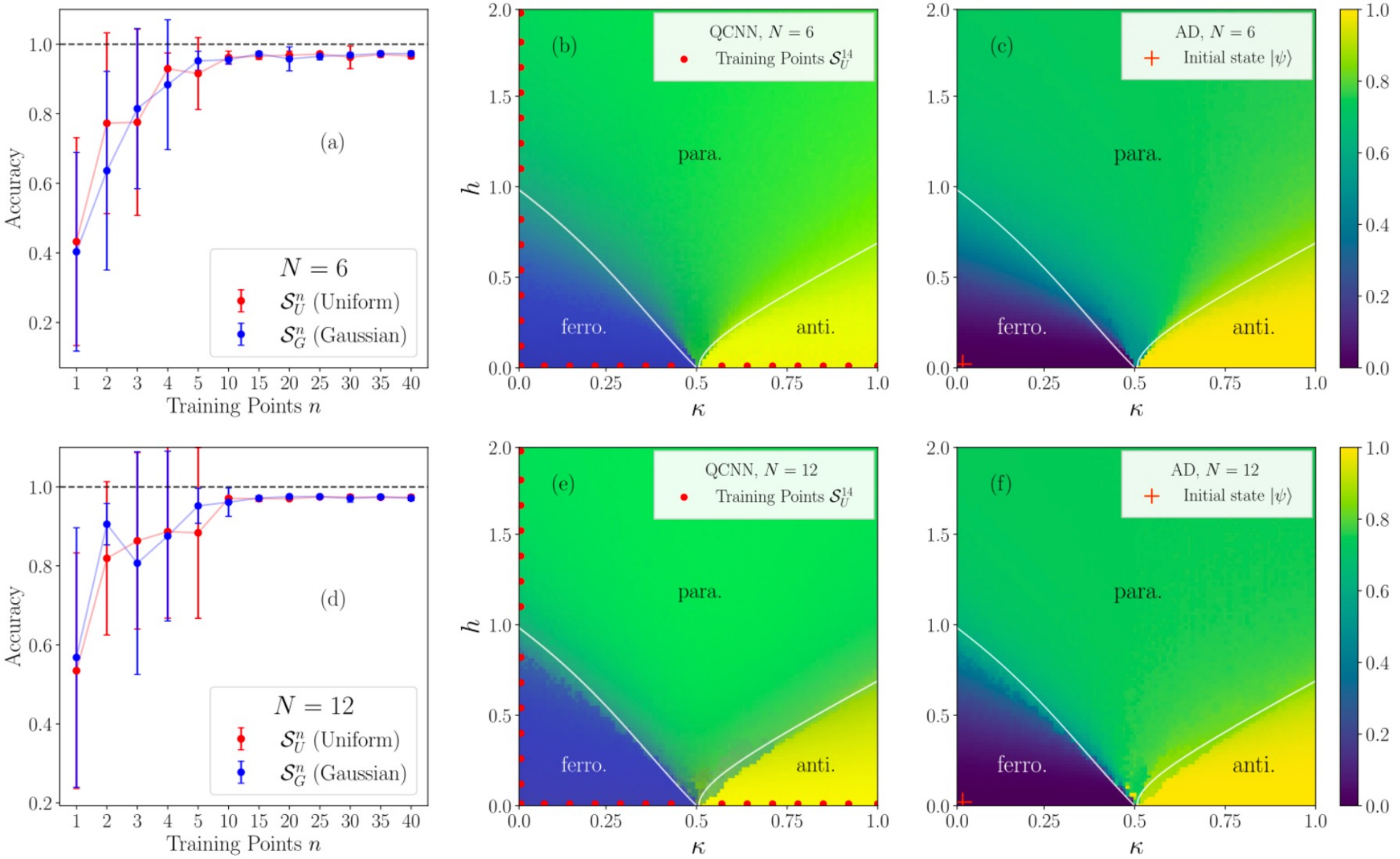
Size of training set

QCNN (95%)

Autoencoder

N = 6

N = 12



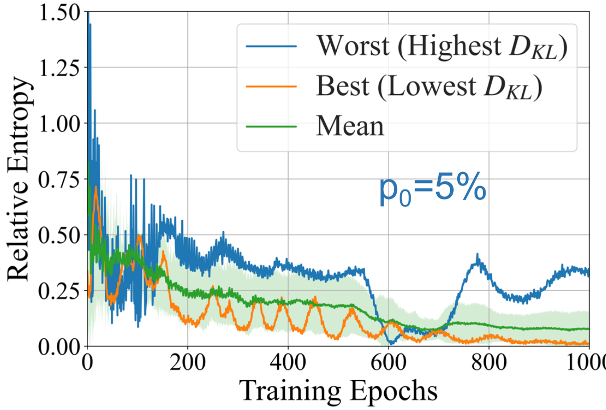
Conclusions

1. Extrapolation from few training data [Caro et al., *Nat Commun* **13**, 4919 (2022)].
2. Performance increases with the system's size.
3. Adresses the bottlneck of needing expensive training labels.
4. QCNN gives quantitative predictions [Banchi et all., Generalization in Quantum Machine Learning: A Quantum Information Standpoint, PRX QUANTUM 2, 040321 (2021)]

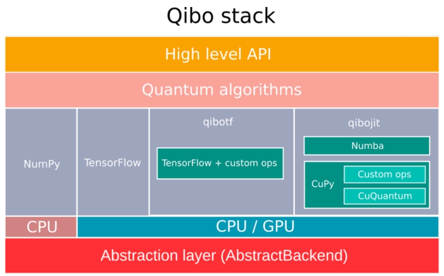
Beyond this…

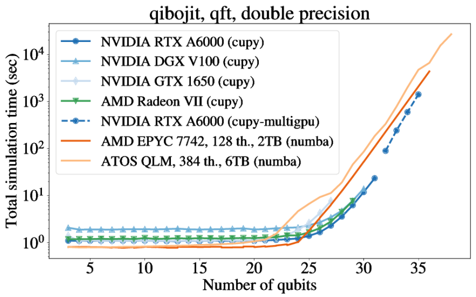
QC @ CERN

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

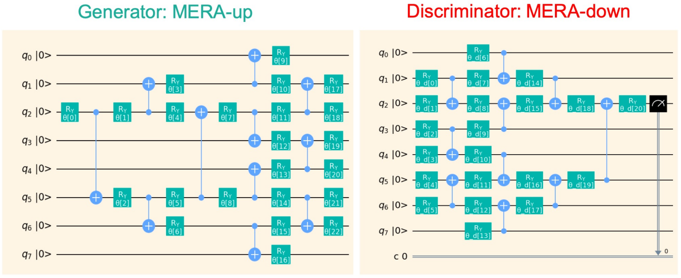


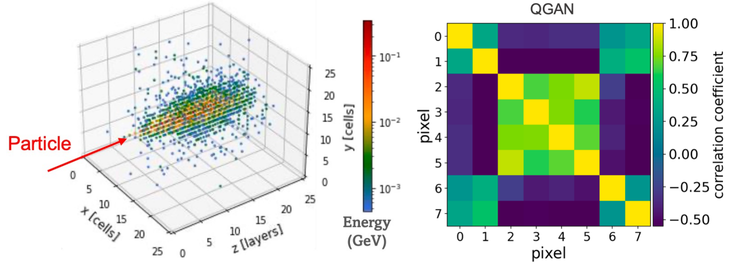
E.Stavros et all., **Quantum simulation with just-in-time compilation**, Quantum 2022



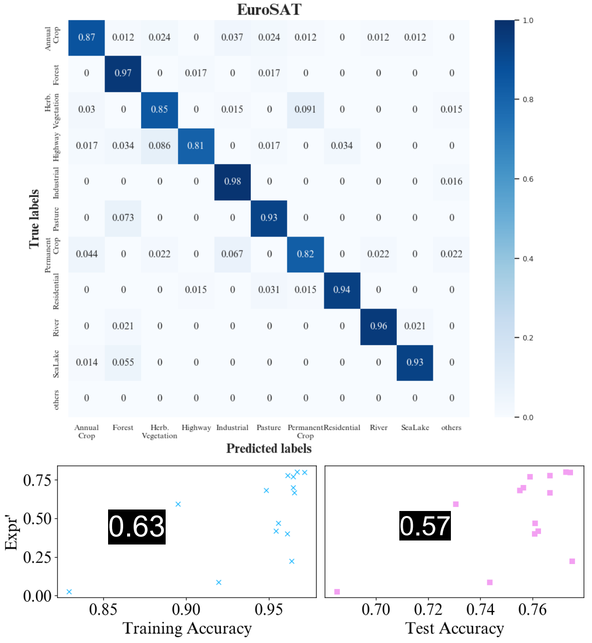


F.Rehm, **Full Quantum GAN Model for HEP Detector Simulations**, ACAT22

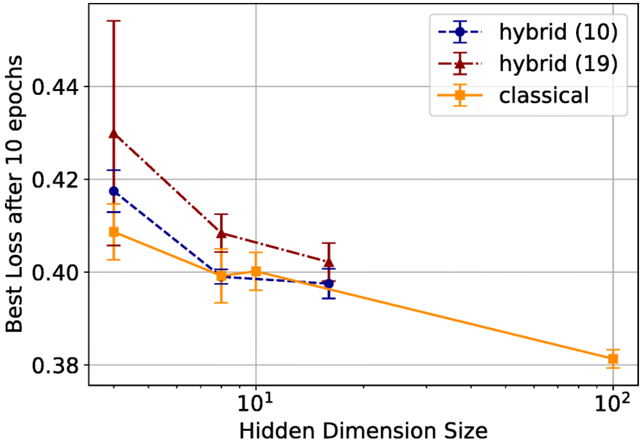




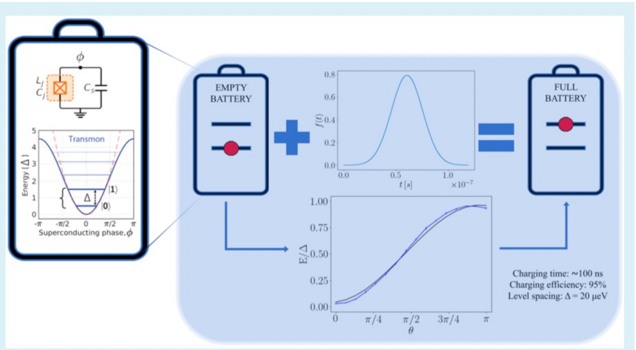
S.Chang, et all, **Hybrid Quantum-Classical Networks for Reconstruction and Classification of Earth Observation Images**, ACAT22



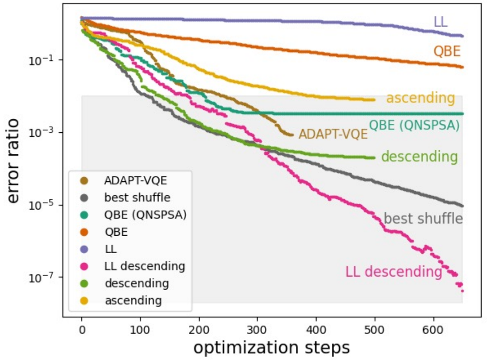
Tüysüz, Cenk, et al. "**Hybrid quantum classical graph neural networks for particle track reconstruction.**" *Quantum Machine Intelligence* 3.2 (2021): 1-20.



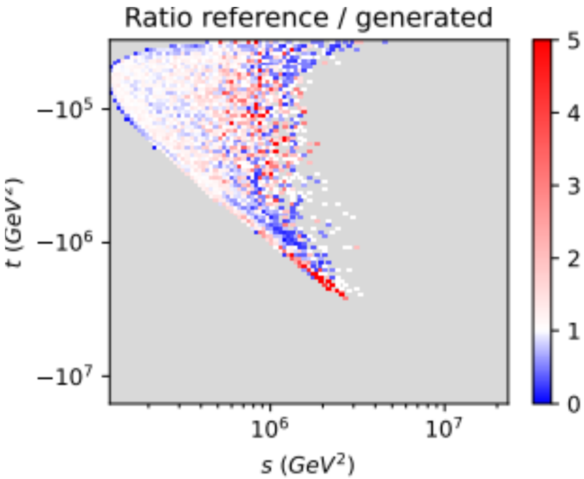
G. Gemme, M. Grossi et al, **IBM Quantum Platforms: A Quantum Battery Perspective**, *Batteries **8**, 43 (2022)*



O. Kiss, **Quantum computing of the 6Li nucleus via ordered unitary coupled cluster**, 10.1103/PhysRevC.106.034325



Bravo-Prieto, Carlos, et al. "**Style-based quantum generative adversarial networks for Monte Carlo events.**" *Quantum 2022*



Exclusion Region for the Higgs mass

- Electroweak fits:

  $m_H < 237$ GeV (95% CL)

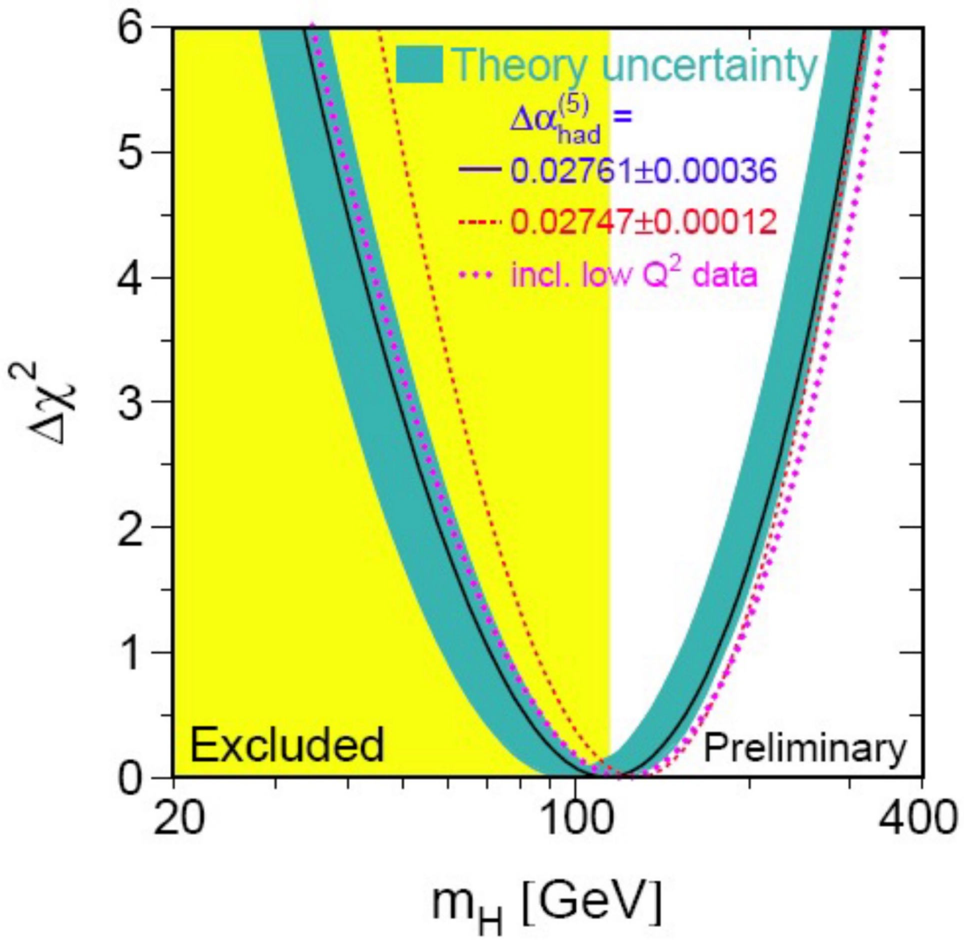
- Theory: self consistency of SM to GUT scale

  $\cong 10^{16}$ GeV

  $130 < m_H < 190$ GeV

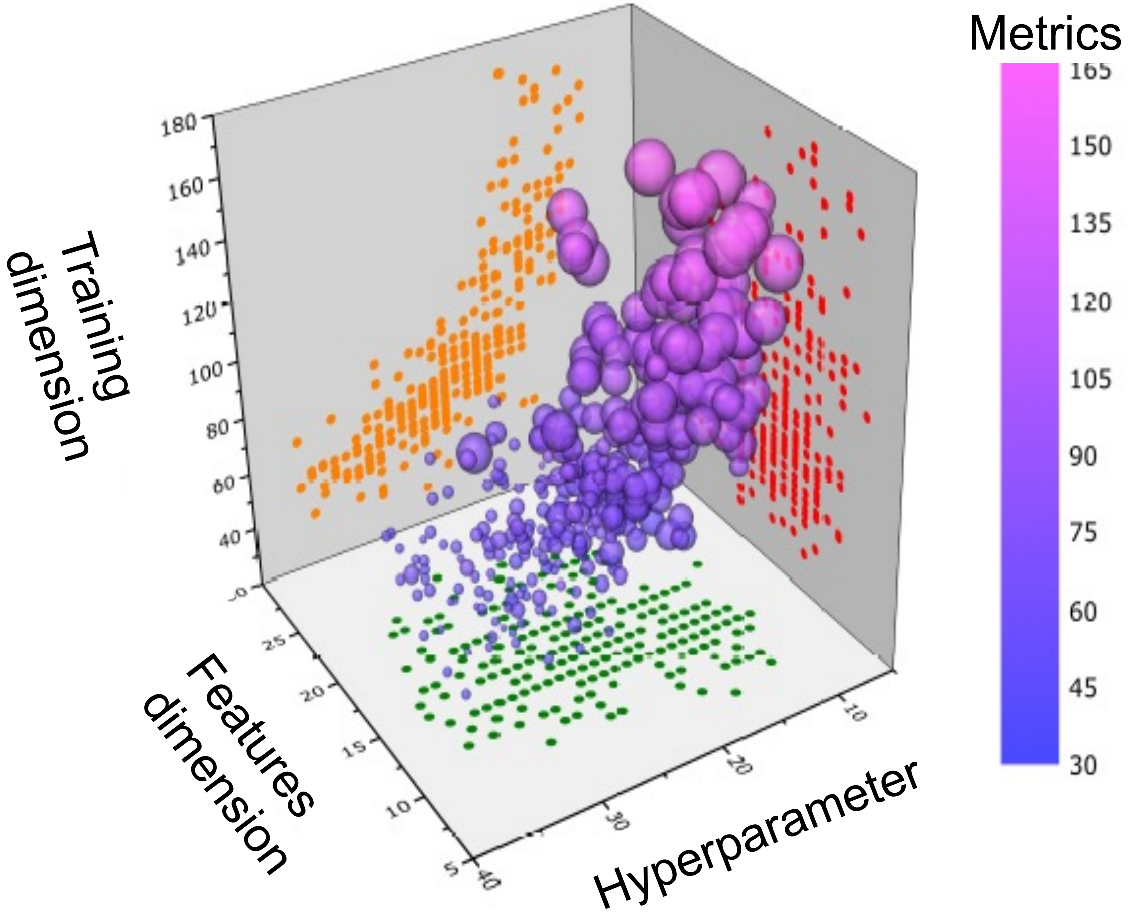
- m_H higher - theory non perturbative,

  m_H lower – vacuum unstable



Exclusion Region for QML in HEP?

- **Classical intractability**: what useful problems can we solve on a quantum computer that we cannot on a classical computer?
- **Innovation**: what new algorithms can we come up with?
- **Computational complexity**: how can we obtain certain speedups?
- Where **QML** is the right solution to our problem?



Thanks!

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