Quantum Machine Learning: from theory to practice @ CERN

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Quantum Computing Scientist

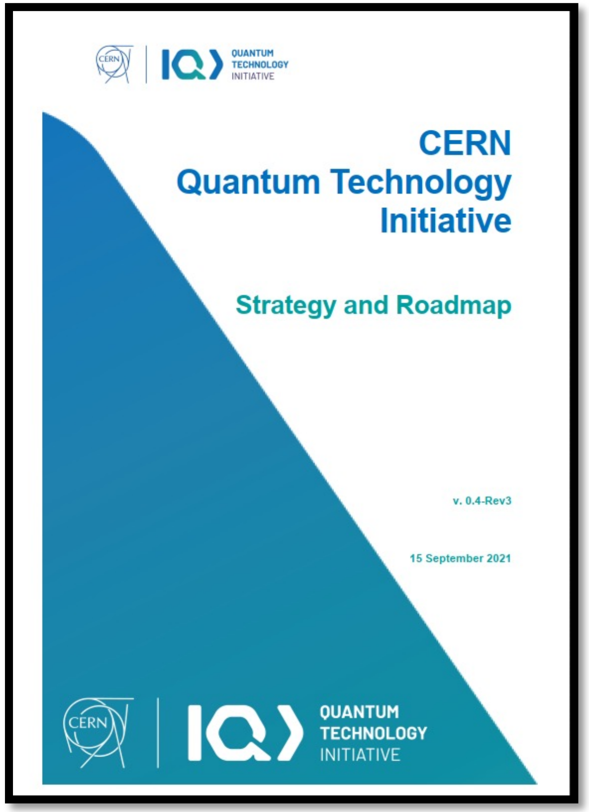
CERN IT Innovation

QUANTUM TECHNOLOGY INITIATIVE

- CERN Quantum Technology Initiative
- QML General Consideration
- Examples from CERN

CERN Quantum Technology Initiative

Discussions about a Quantum Technology Initiative took place in 2020 with representatives of quantum initiatives in the CERN Member States, the CERN community, the Worldwide LHC Computing Grid, the CERN Scientific Computing Forum, with LHC experiments and the HEP Software Foundation


QUANTUM TECHNOLOGY INITIATIVE

CERN
Quantum Technology
Initiative

Strategy and Roadmap

v. 0.4-Rev3

15 September 2021

QUANTUM
TECHNOLOGY
INITIATIVE

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

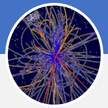
T1 - Scientific and Technical Development and Capacity Building

T3 - Community Building

T2 - Co-development

T4 - Integration with national and international initiatives and programmes

Scientific Objectives



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

CERN IBM Quantum Hub

Since 2021 CERN is a “Hub Member” in the IBM Quantum Network and has welcome two new members in 2022

A project-based hub dedicated to quantum computing applications to fundamental physics research, computational chemistry, computational biology, and related fields

CERN

INFN Istituto Nazionale di Fisica Nucleare

iit ISTITUTO ITALIANO DI TECNOLOGIA

International Conference on Quantum Technologies for High-Energy Physics (QT4HEP22)

CERN | QUANTUM TECHNOLOGY INITIATIVE

1–4 Nov 2022
CERN
Europe/Zurich timezone
There is a live webcast for this event.

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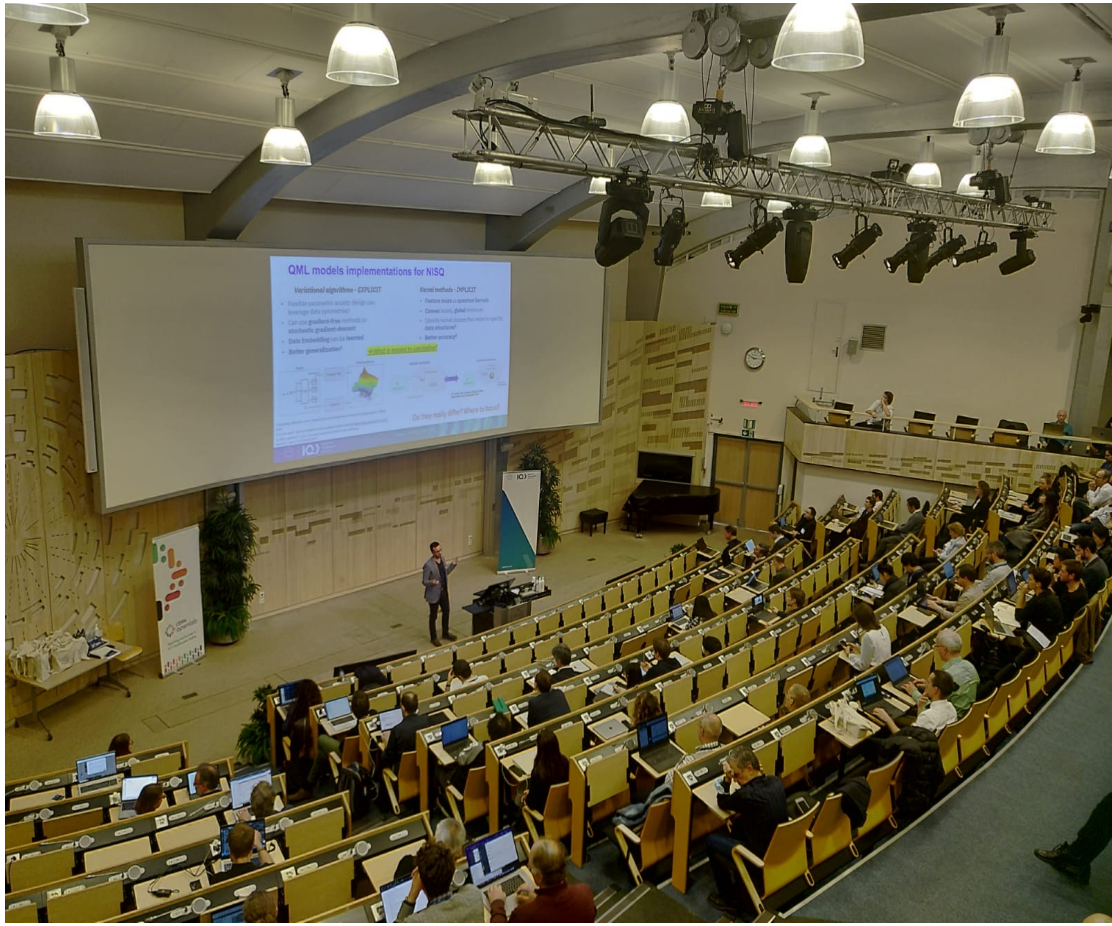
Contact

QT4HEP-conference@c...

Registration deadline extended until Friday, 28 October for the International Conference on Quantum Technology for High-Energy Physics, which will be hosted at CERN on 1–4 November 2022.

Following CERN's successful workshop on quantum computing in 2018, this is the first edition of the #QT4HEP conference taking place to further investigate the nascent quantum technology and its great promise to support scientific research.

Bringing the whole community together, we aim to foster common activities and knowledge sharing, discuss the recent developments in the quantum science field and keep looking for activities within HEP — and beyond — that can most benefit from the application of quantum technologies.

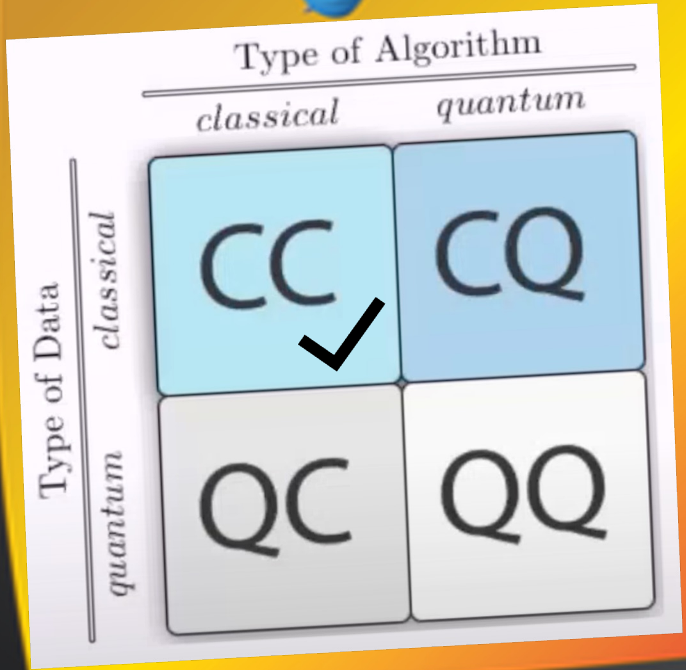


Computing & Algorithms

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

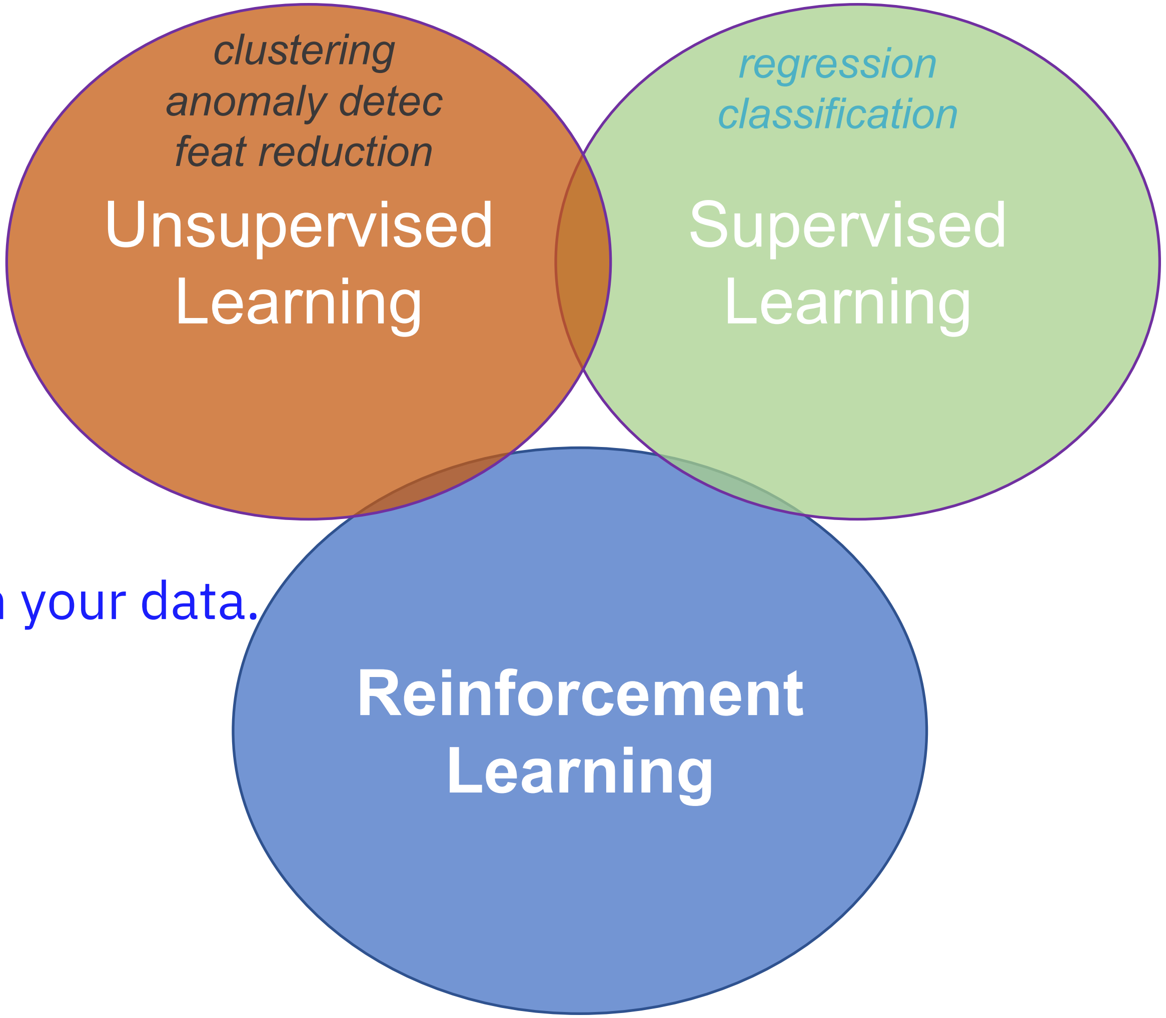
Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

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



- CERN Quantum Technology Initiative
- **QML General Consideration**
- Examples from CERN

You got your data: what's next?



Supervised ML

Labeled data, i.e., data with defined output.

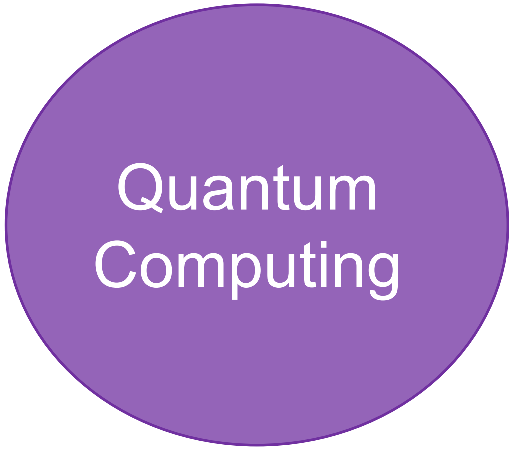
A model is trained giving this data and you have direct evaluation.

Unsupervised ML

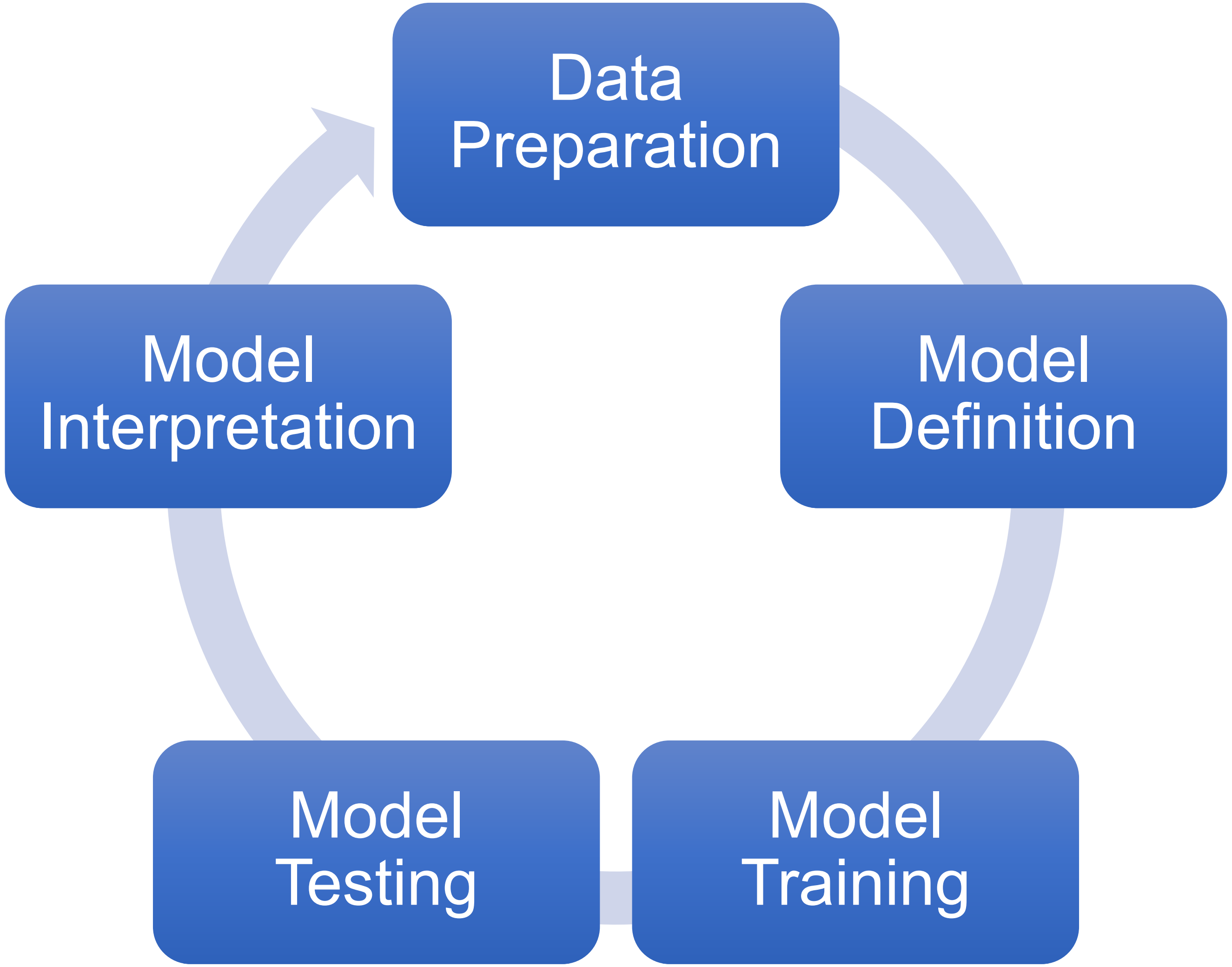
Unlabeled data.

ML finds patterns in your data.

Indirect evaluation.



Machine Learning Model Lyfecycle

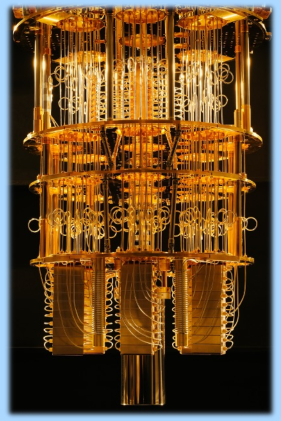


Quantum Machine Learning Model Lyfecycle

The quantum advantage of many known QML algorithms is impeded by an input or output bottleneck

Data Preparation

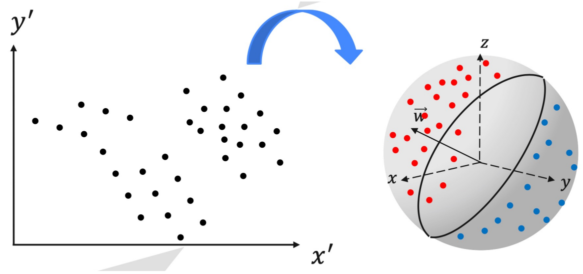
Model Interpretation



Model Definition

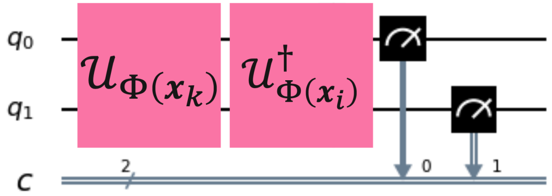
Model Testing

Model Training

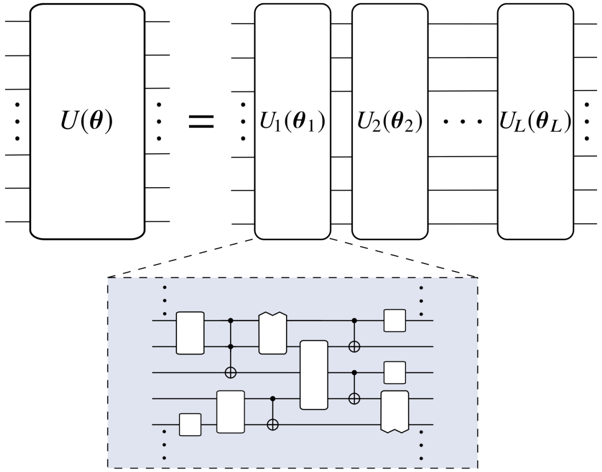


Data Reduction
Data Encoding [1,2,3]

Read Out



Trainability (BP…)



[1] Robust data encodings for quantum classifiers, Ryan LaRose and Brian Coyle, Phys. Rev. A 102, 032420

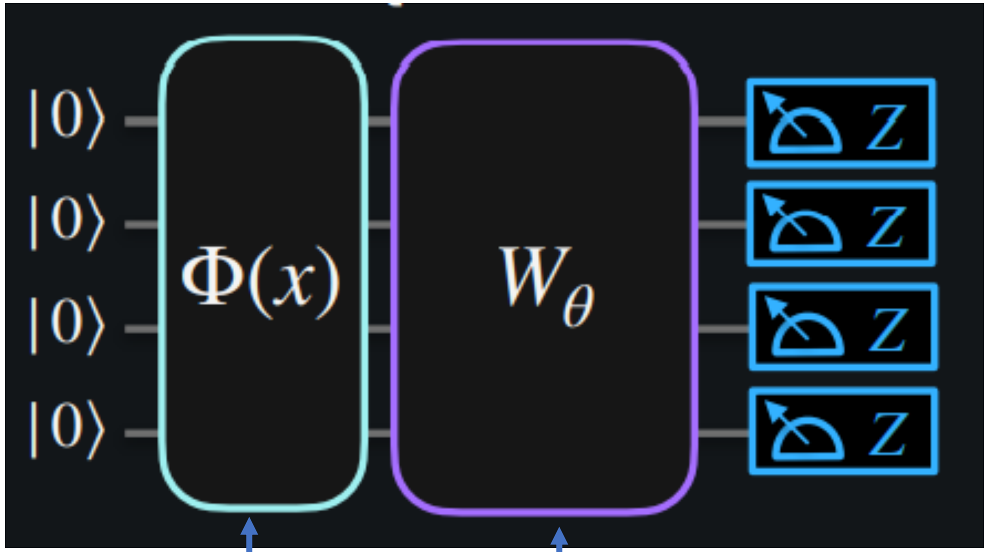
[2] Quantum convolutional neural network for classical data classification, https://arxiv.org/pdf/2108.00661.pdf

[3] Quantum Support Vector Machines for Continuum Suppression in B Meson Decays, https://arxiv.org/abs/2103.12257

QML models implementations for NISQ

Variational algorithms - EXPLICIT

- Flexible parametric ansatz: design can leverage data symmetries[1,2]
- Can use **gradient-free** methods or **stochastic gradient-descent**
- **Data Embedding** can be **learned**
- **Better generalization[2,3]**



Feature map Parametrized circuit

A linear classifier in the quantum feature space!

1-A. Bogatskiy et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020
2-J. Meyer et al "Exploiting symmetry in variational quantum machine learning", https://arxiv.org/abs/2205.06217
3-S.Jerbi at all., Quantum Machine Learning Beyond Kernel Methods https://arxiv.org/abs/2110.13162
4- Glick, Jennifer R., et al. "Covariant quantum kernels for data with group structure." arXiv:2105.03406 (2021)

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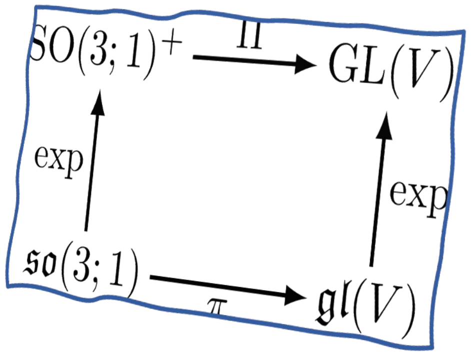
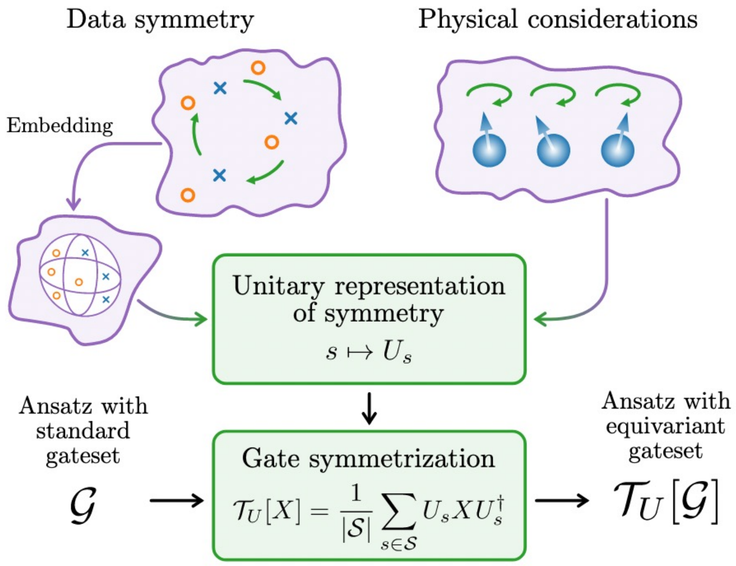
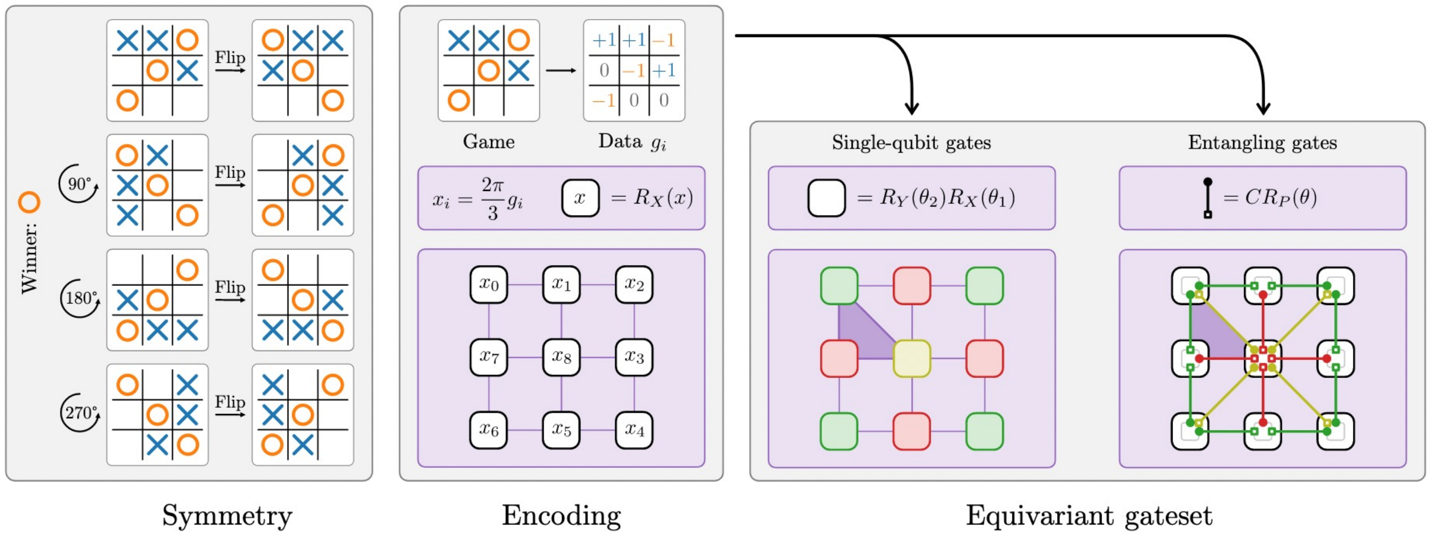


https://github.com/fizisist/LorentzGroupNetwork



A unitary representation of a symmetry group S can arise from data symmetries when the data points are suitably encoded or alternatively from physical considerations of a variational problem[2].



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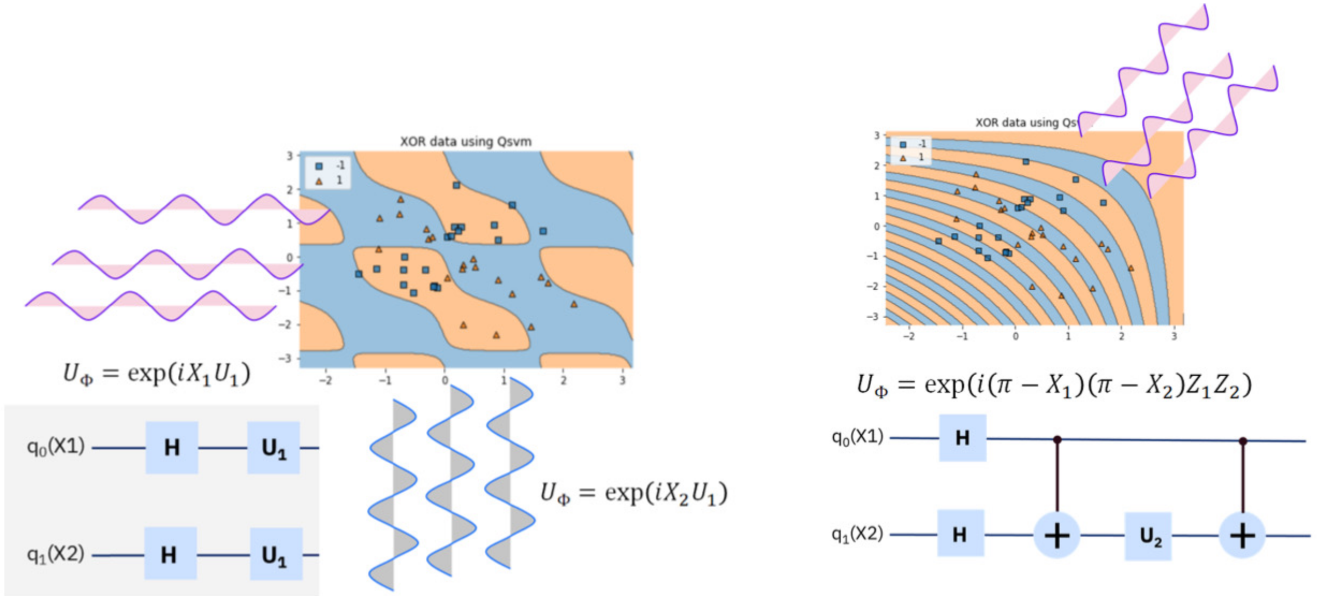
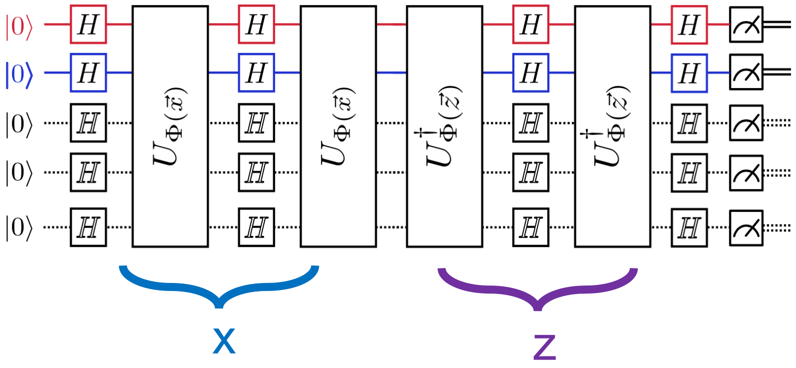
QML models implementations for NISQ



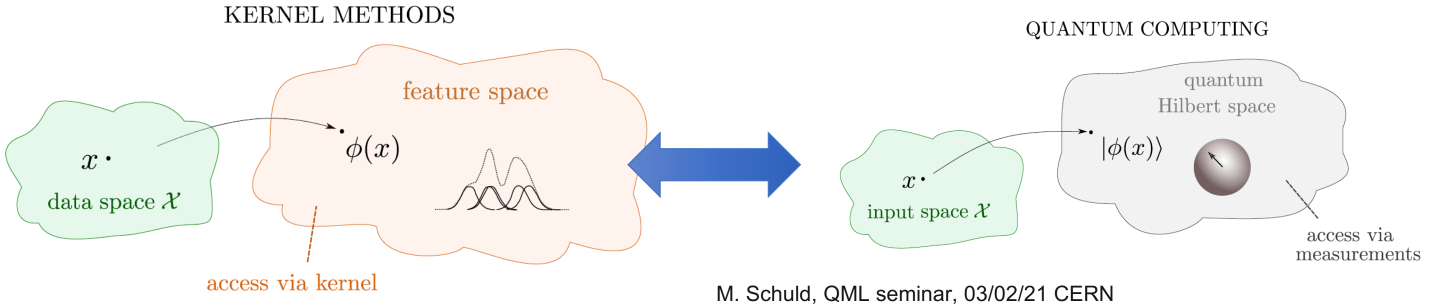
(a) (b)

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]



$$|\langle \Phi(\vec{x}) | \Phi(\vec{z}) \rangle|^2 = |\langle 0^n | \mathcal{U}^\dagger_{\Phi(\vec{x})} \mathcal{U}_{\Phi(\vec{z})} | 0^n \rangle|^2$$



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

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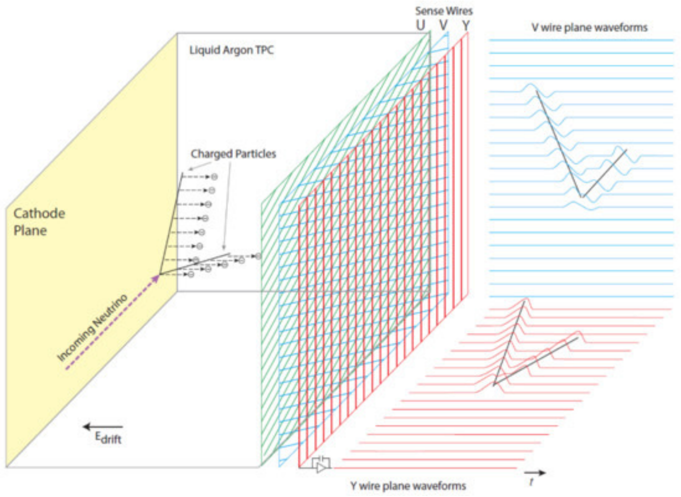
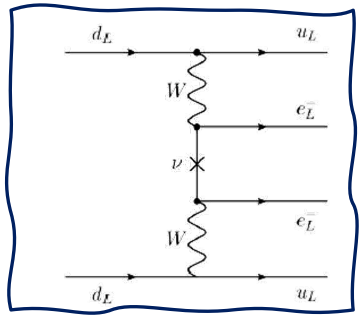
- QML General Consideration
- **Examples from CERN**

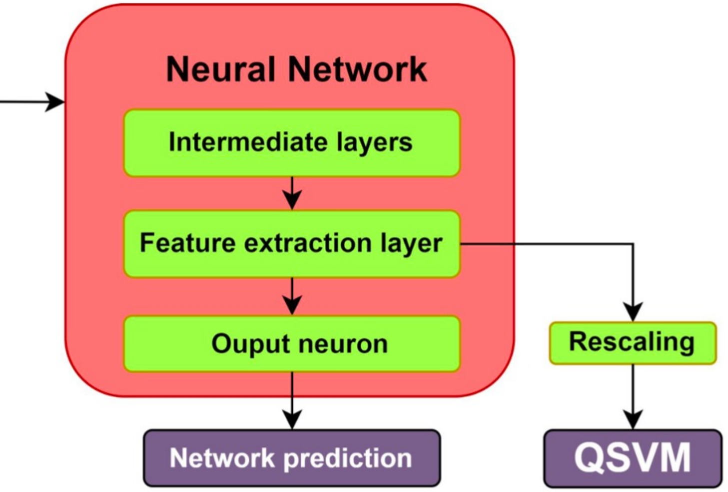
Roberto Moretti et al. , https://agenda.ciemat.es/event/404

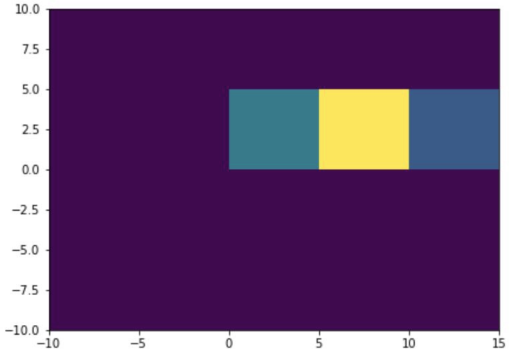
Double beta decay search at DUNE

- Evidence of **ν** as maiorana particles and lepton number violation
- Visible at Dune Liquid Xe TPC
- Largest background is single β emission (^{42}Ar, neutrons, solar neutrinos, etc..) + ννββ
- MC-based study with realistic **detector spatial resolution (5mm)**
- DATA PREPARATION:
  CNNs and **Transformers (Attention Network)**







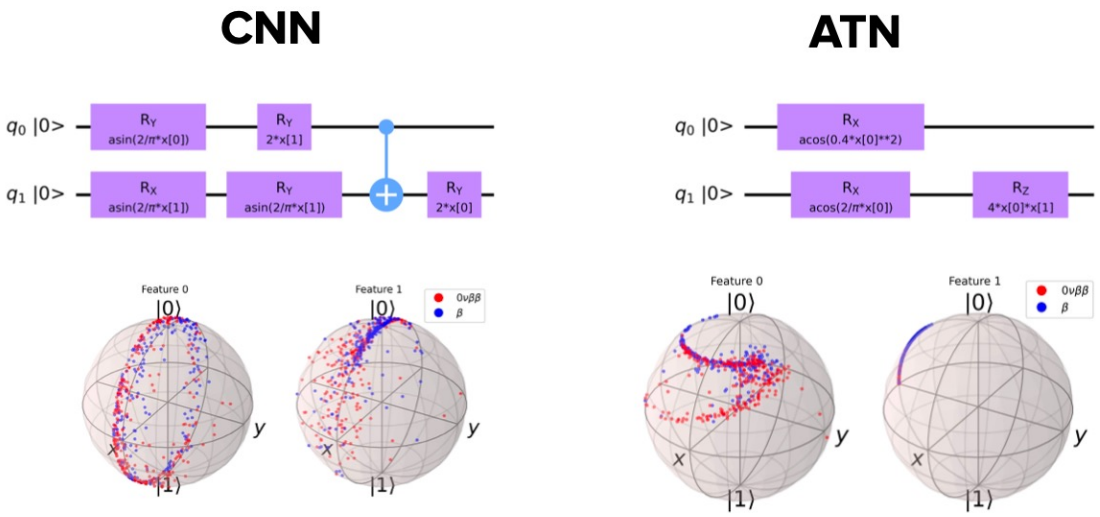


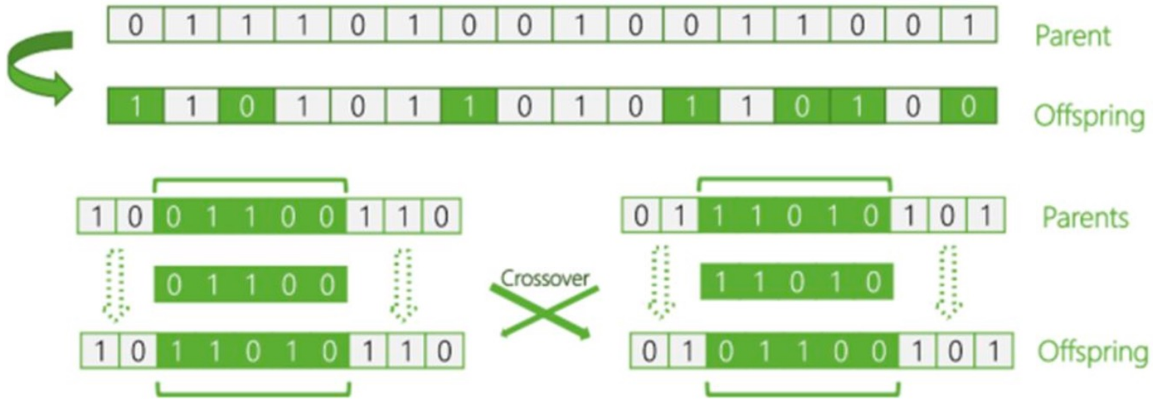
Picture from: https://www.mdpi.com/2076-3417/11/6/2455/htm#

Double beta decay search at DUNE

QML Challenge: achieving a good β vs ββ separation

- Comprehensive study on **QSVM performance**
  - **Kernels**
  - **Input features**
  - **Circuit depth**
- Kernel design via **genetic optimisation**
  - Binary representation of the feature map circuit
  - Test on IBM *Lagos*

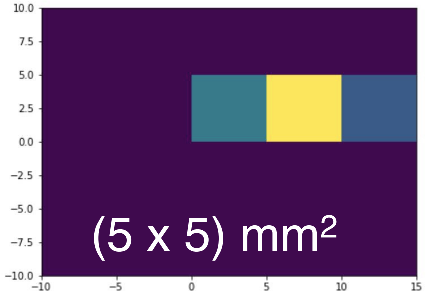


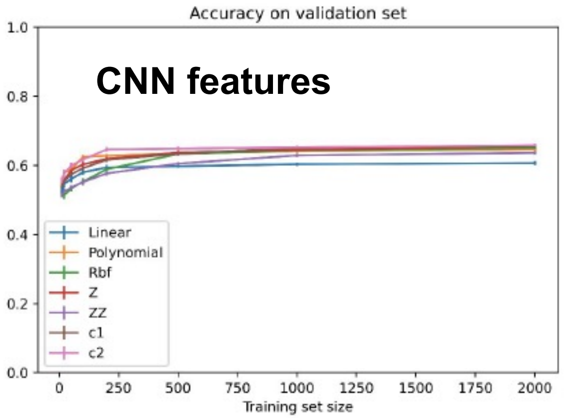


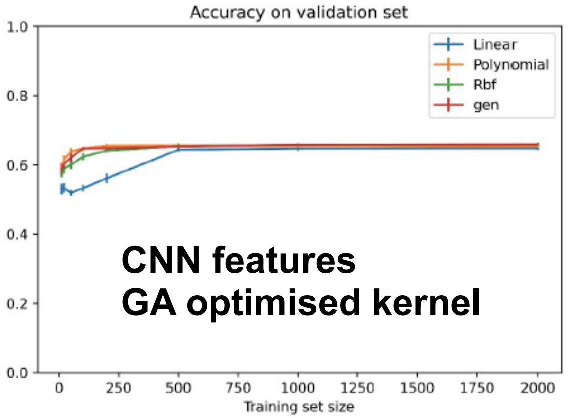
Roberto Moretti et al. , https://agenda.ciemat.es/event/4042/

Some results

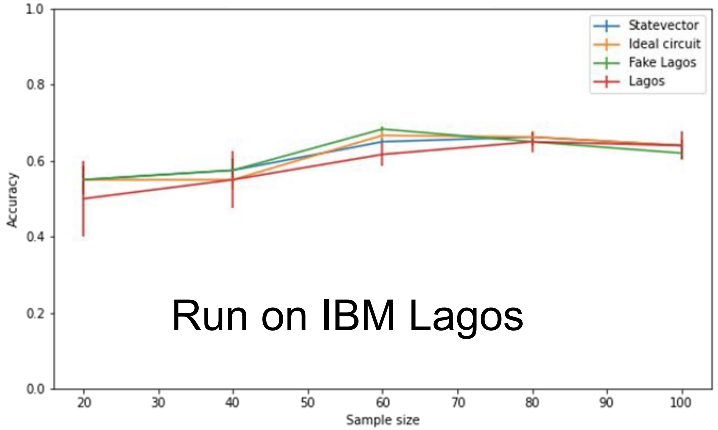
- QSVM is **as good as** classical
- Increasing number of qubits does not improve accuracy at convergence: can lead to overfitting
- Results seems driven by the **feature map performance**



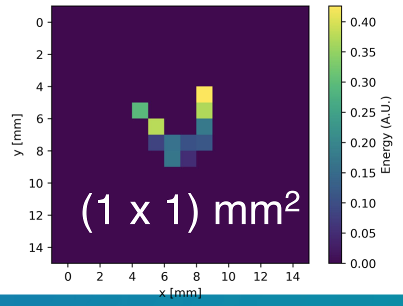


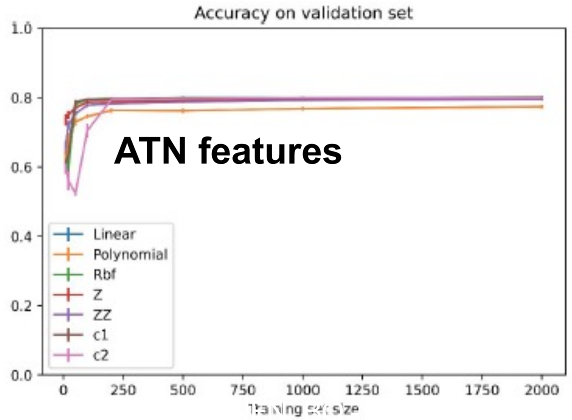


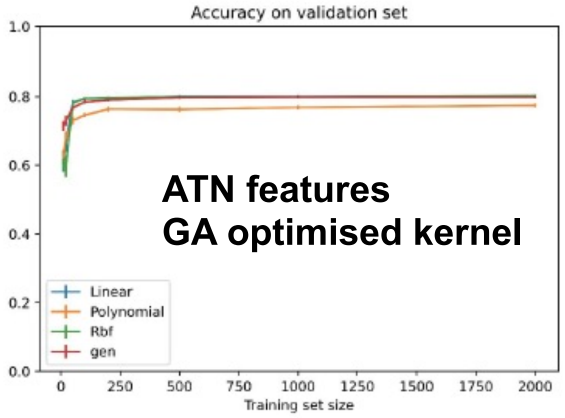
ZZ feature map



Need **higher spatial** resolution resolution !







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

geometry test

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

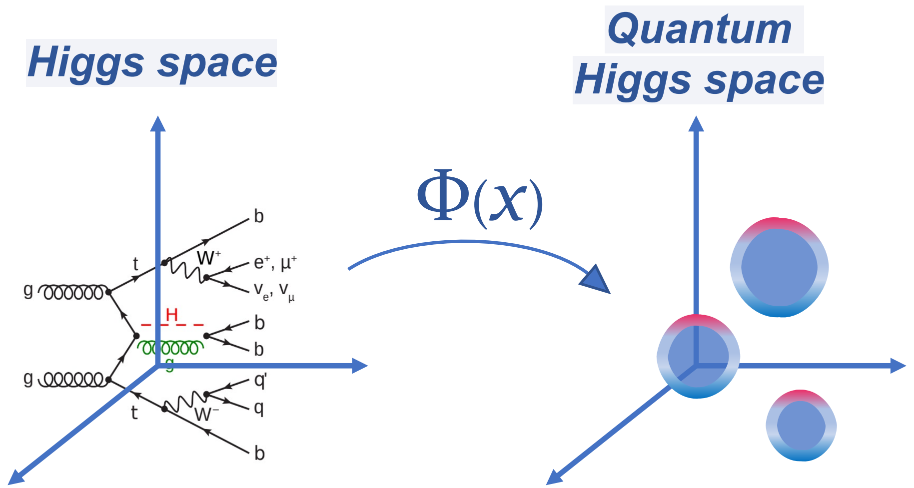
Constraints:

- 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
https://quask.readthedocs.io/en/latest/#

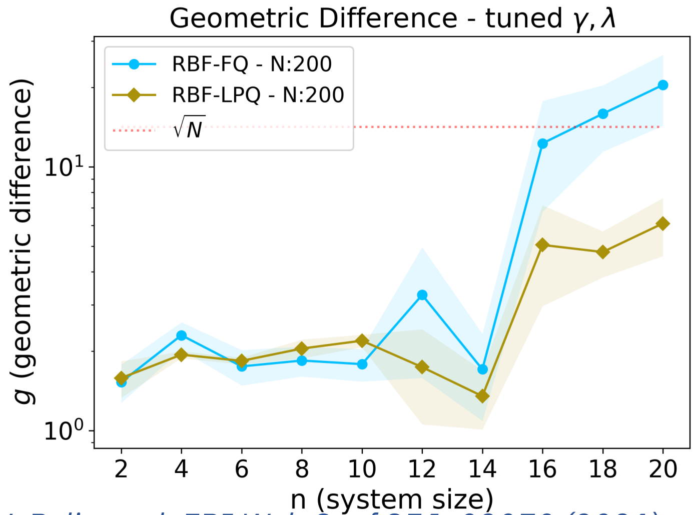
Interpretation in HEP

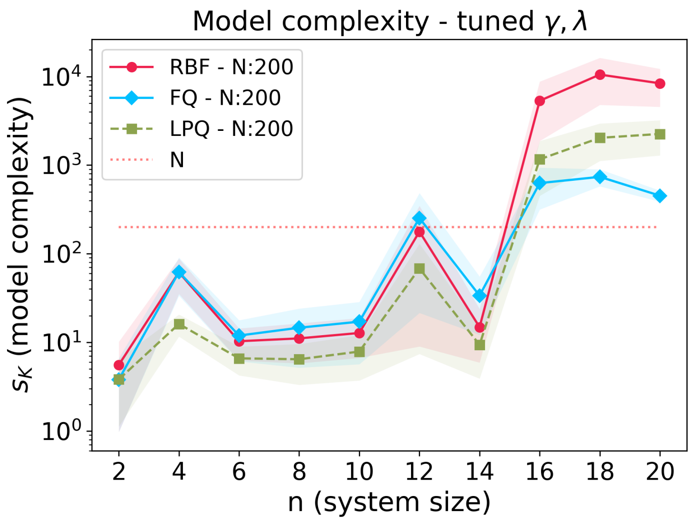
- From general observation:
  - High number of qubits → High expressivity: data lost in the Hilbert space
  - $d \approx N$ → Low generalization power

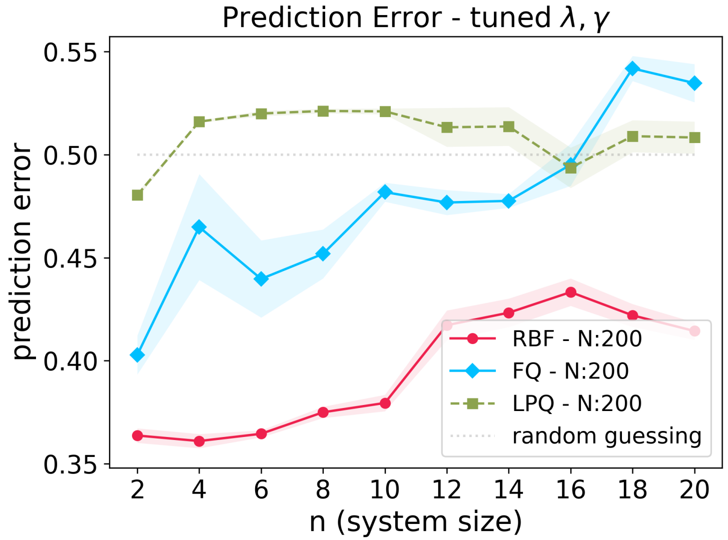


- HEP observation:
  - Quantum kernels have moderate g_{QC} → Worse performance than the classical counterpart, no QA

EXAMPLE: QSVM for the tt →H →(bb) event classification [2,3]

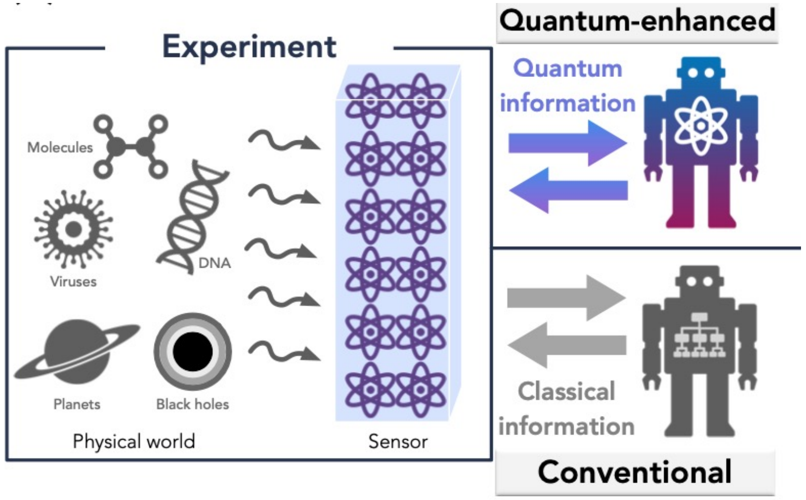






[2] V. Belis et al, EPJ Web Conf **251**, 03070 (2021)
[3] F.Di Marcantonio et al., in preparation

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)

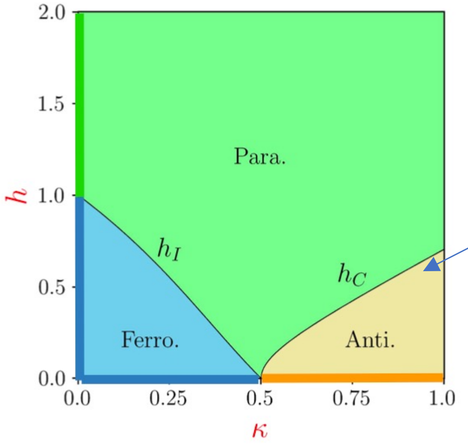
QML for OO Generalization

- **Train in easy (integrable) subregions**
- **Generalize to a full model[1]**
- Model: Axial Next Nearest Neighbor Ising (ANNNI) Hamiltonian:

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

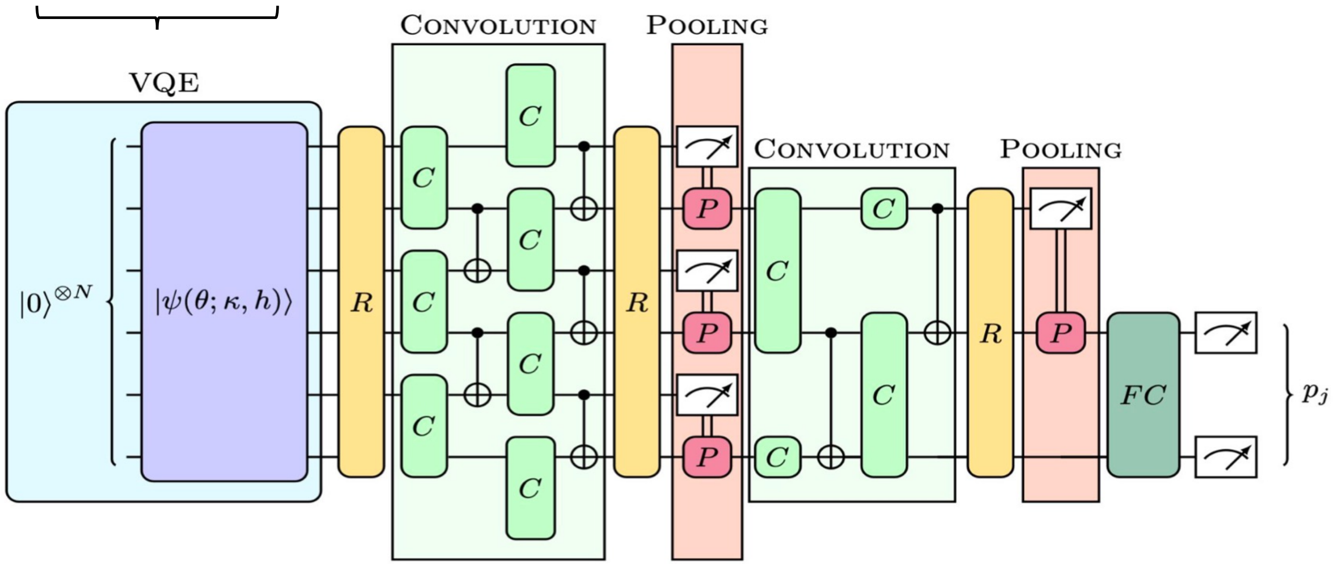
Senk, *Physics Reports*, **170**, 4 (1988)

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)

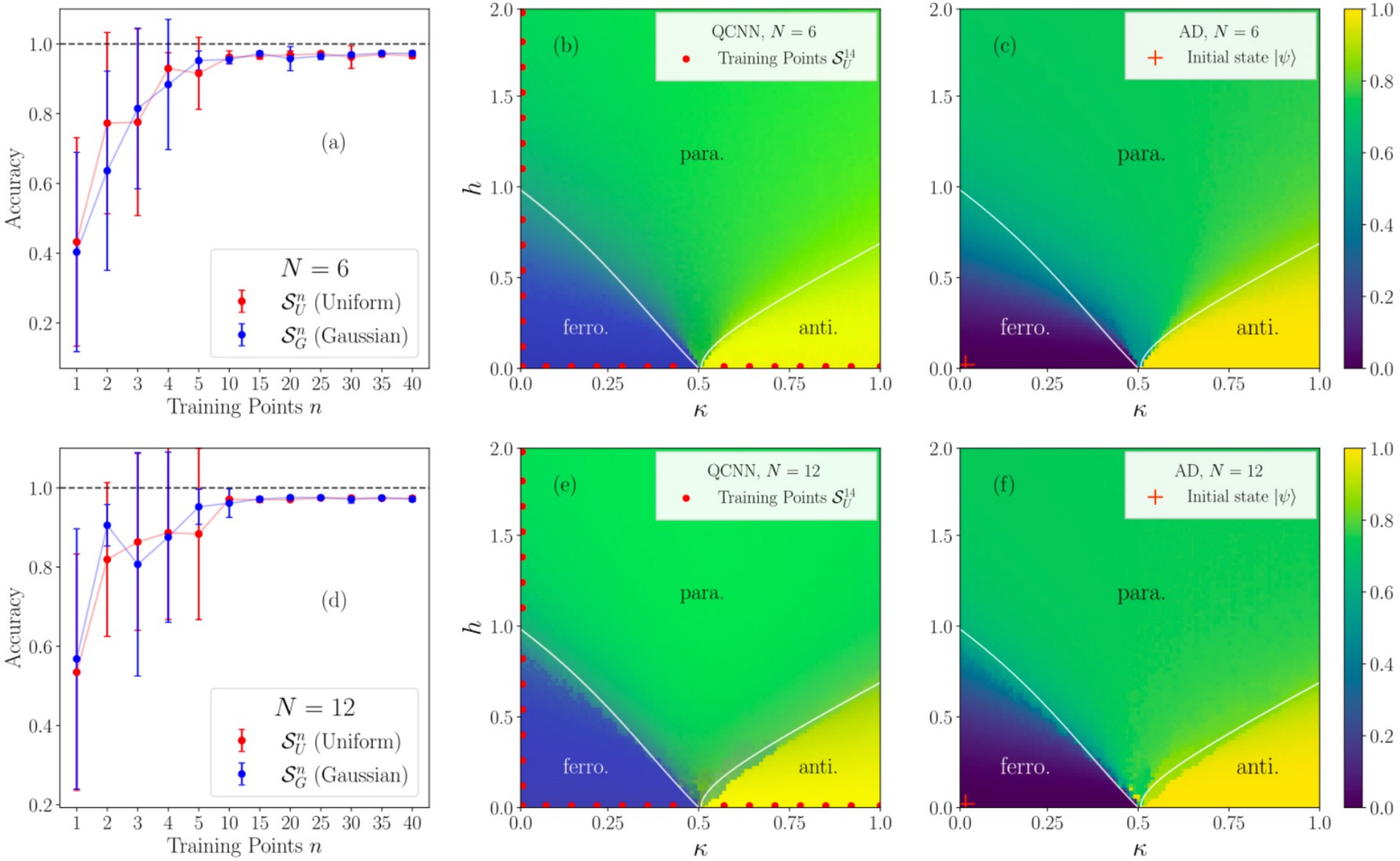
Learn a similarity function between the data.

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

Size of training set QCNN (95%) Autoencoder

N = 6

N = 12



Conclusions

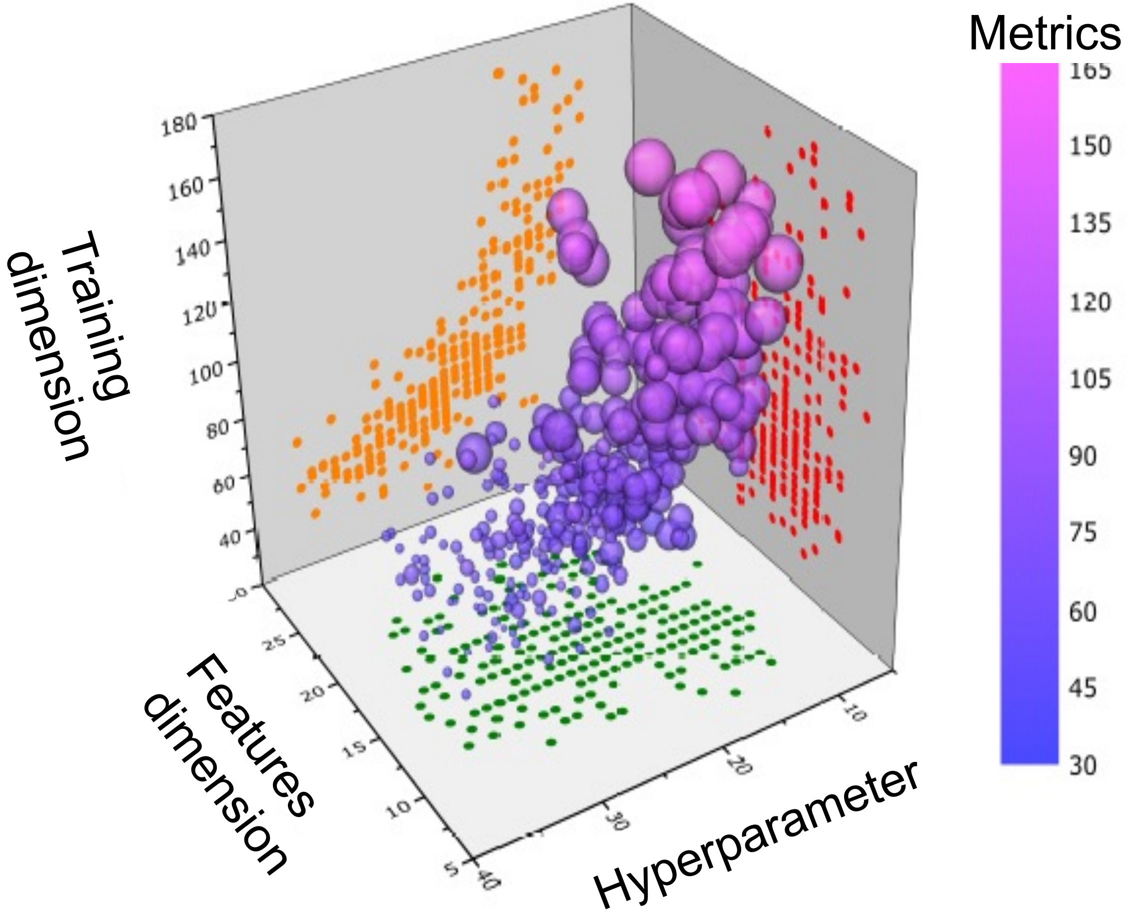
1. Out of Distribution Generalization [M..Caro et al., Out-of-distribution generalization for learning quantum dynamics, https://arxiv.org/abs/2204.10268]
2. Performance increases with the system's size.
3. Adresses the bottlneck of needing expensive training labels.
4. QCNN gives quantitative predictions [Banchi et all., Generalization in Quantum Machine Learning: A Quantum Information Standpoint, PRX QUANTUM 2, 040321 (2021)]

Characterize Quantum Advantage

- Classical machine learning models can often compete or outperform existing quantum models even on data sets generated by quantum evolution
- Large quantum Hilbert space in existing quantum models can result in significantly inferior prediction performance compared to classical machines: expressivity of QML hinder generalization
- We need a methodology for assessing the potential for quantum advantage in prediction on learning tasks
- Are there alternative research questions beyond the goal of beating classical machine learning?

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?



THANK YOU

michele.grossi@cern.ch

QUANTUM MACHINE LEARNING

2023