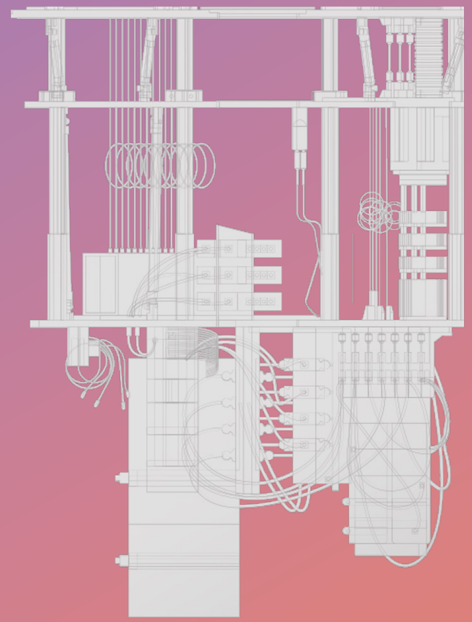
Quantum Machine Learning Techniques for Data Analysis in High-Energy Physics

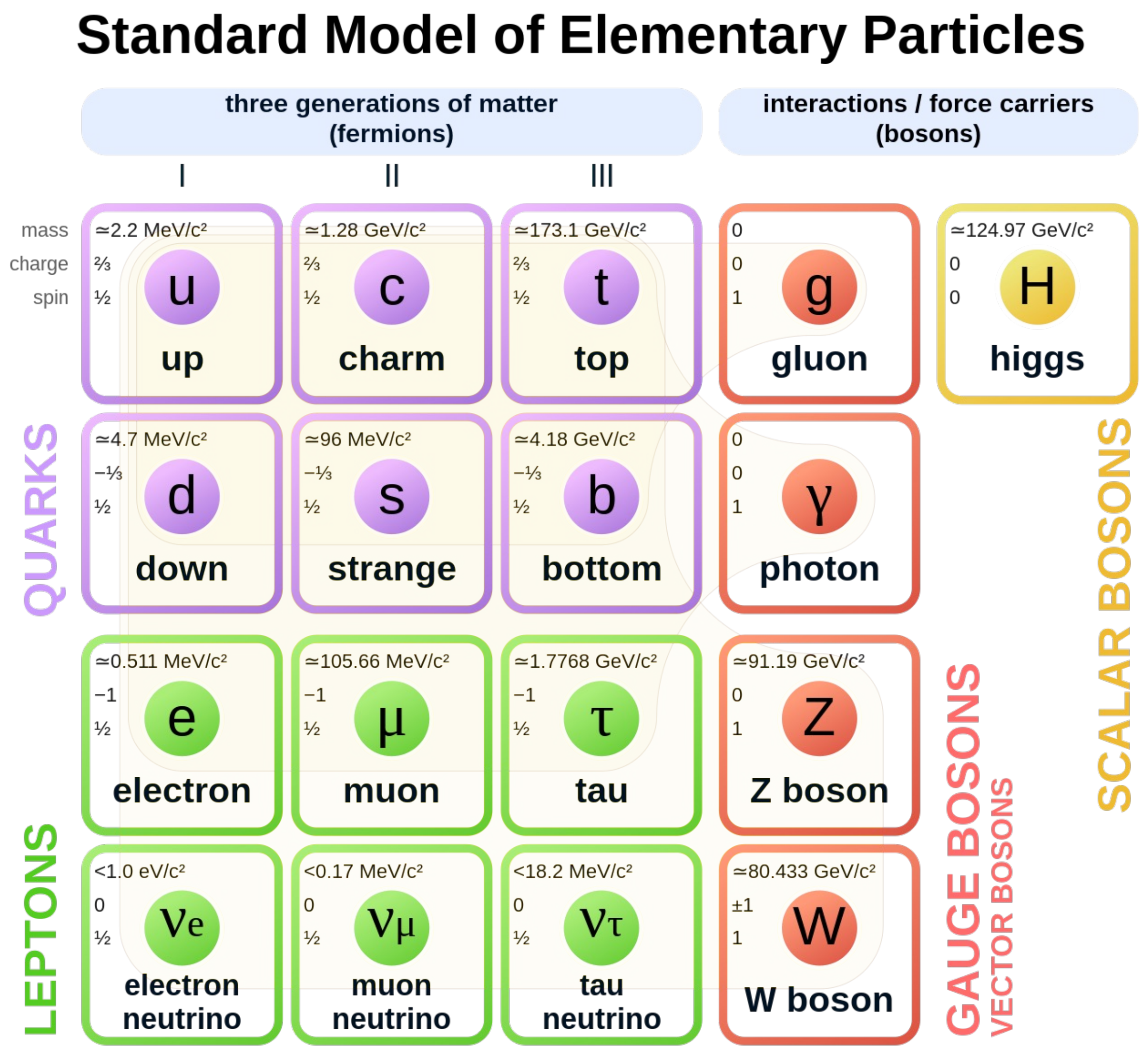


Andrea Delgado (she/her/ella)

Oak Ridge National Laboratory

High-Energy Physics

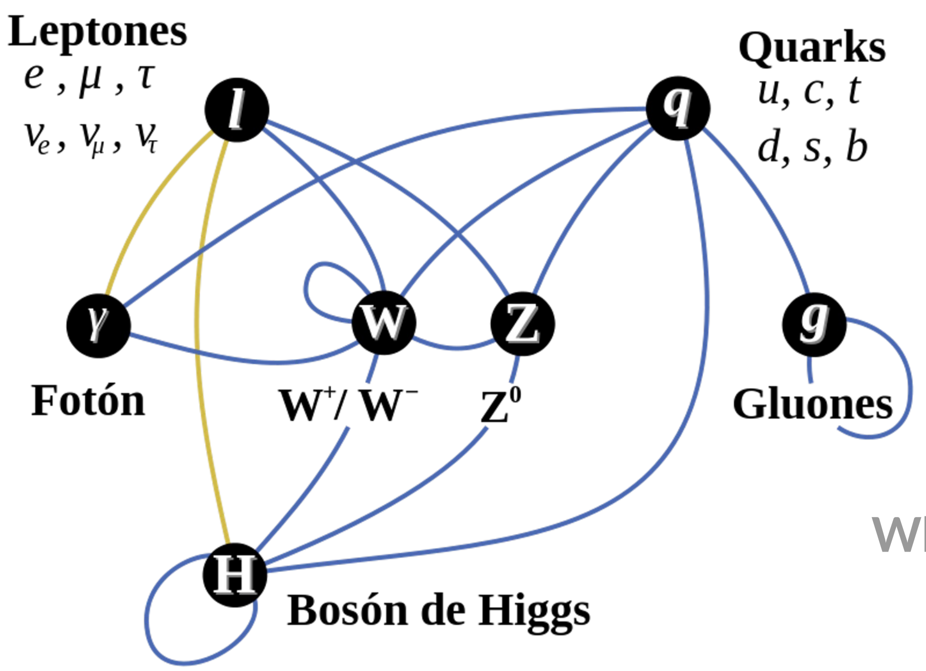
- ★ Seeks to understand matter and its interactions at the **fundamental level**.
- ★ The **standard model (SM)** is currently the best description that we have about the subatomic world.
- ★ Within the SM context, the interaction between the fundamental blocks of matter – the **leptons** and **quarks** – are mediated by the four **fundamental forces**.



The standard model has been extremely successful theory, but…

Why do neutrinos have mass?

Is there a particle associated with gravity?



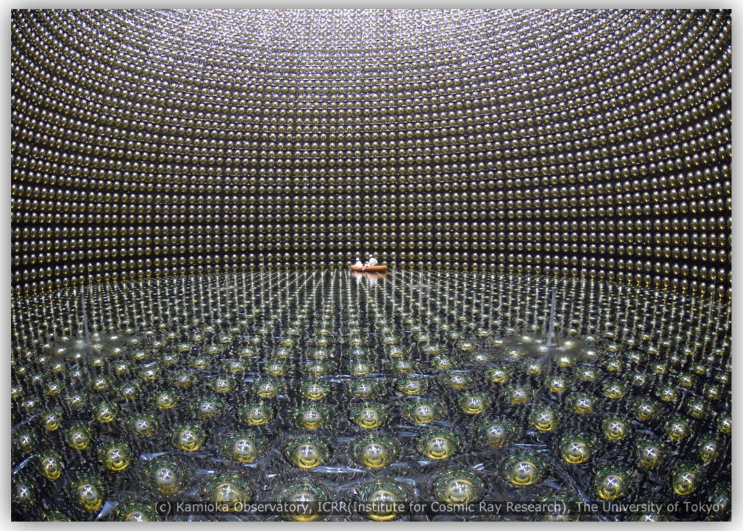
Why are there three generations of matter?

What is dark matter?

Why does the Higgs boson has a mass of 125 GeV?

… it is incomplete

Experimental High-Energy Physics



Super-Kamiokande (Neutrino Observatory))

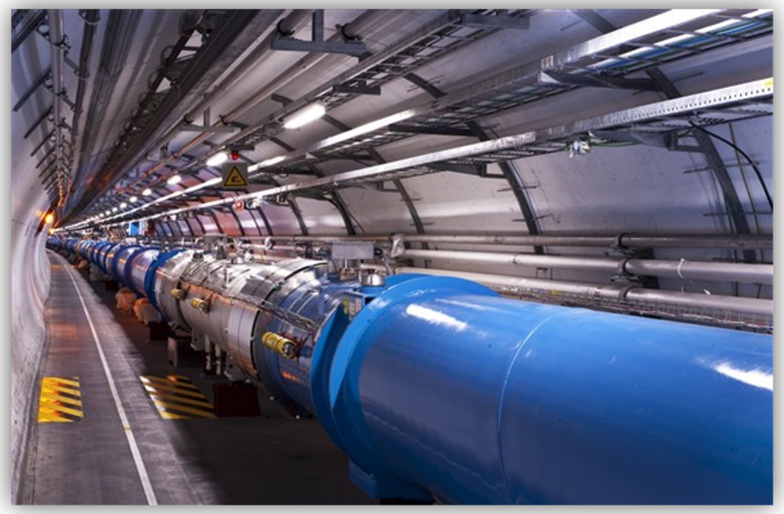
Japan, underneath mount Ikeno

First evidence of neutrino oscillation

Tevatron (Particle Accelerator)

Illinois, USA

Top quark discovery



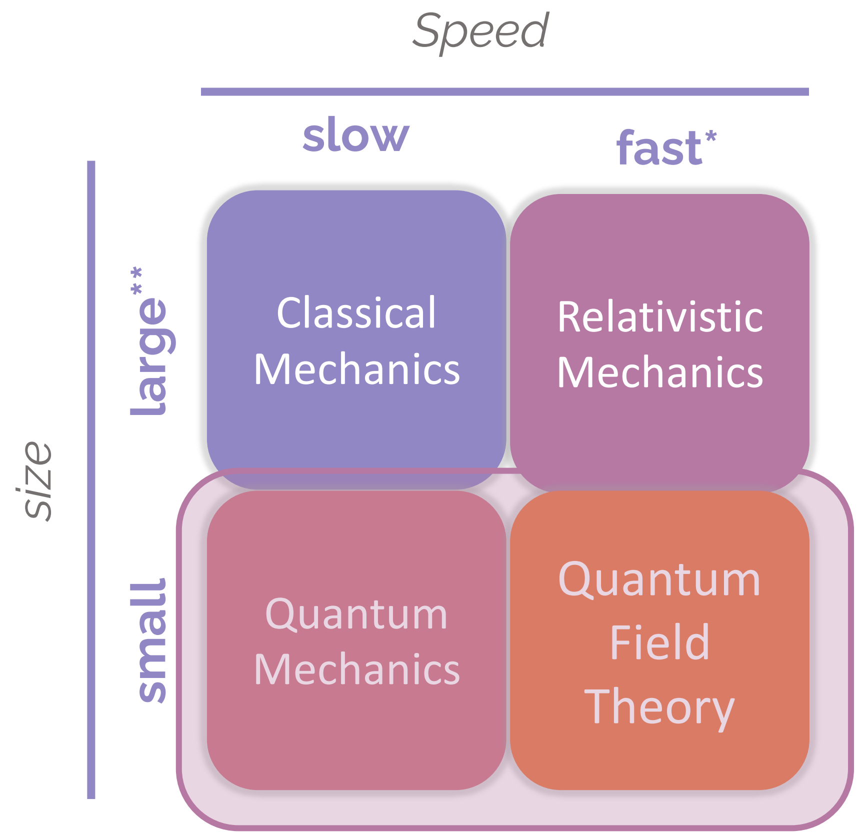
Large Hadron Collider (Particle Accelerator)

Switzerland

Higgs boson discovery

Large, complex datasets that pose a challenge to conventional information processing systems – how **can we speed up some computational tasks?**

A deeper connection to the quantum world



Think about chemistry, molecules

Think about quarks and gluons.

- fast = close to speed of light

** small = close to the radius of an atom

These quantum objects also posses some interesting properties…

such as entanglement, superposition, interference

features that make it difficult to study with current information processing techniques (lattice QCD, many-body problems).

So what about using quantum computers to study quantum systems?

“ Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy”

– *Richard Feynman*

A simple, yet powerful idea.

HIlbert space is a big place!

Carlton Caves

With 275 qubits, we can represent more basis/computational states than the number of atoms in the observable universe.

$$2^{275}$$

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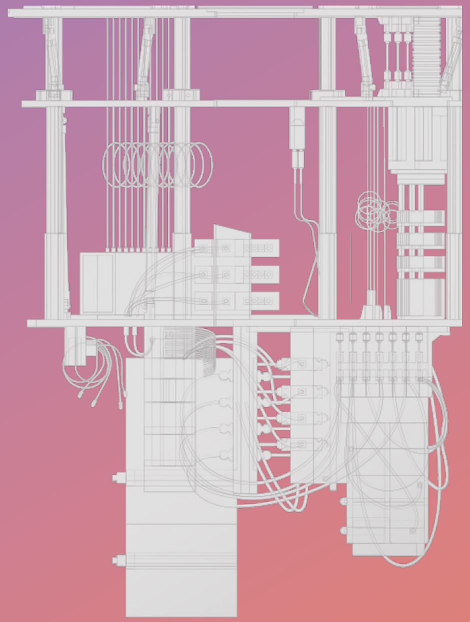
Carlton Caves

With 275 qubits, we can represent more basis/computational states than the number of atoms in the observable universe.

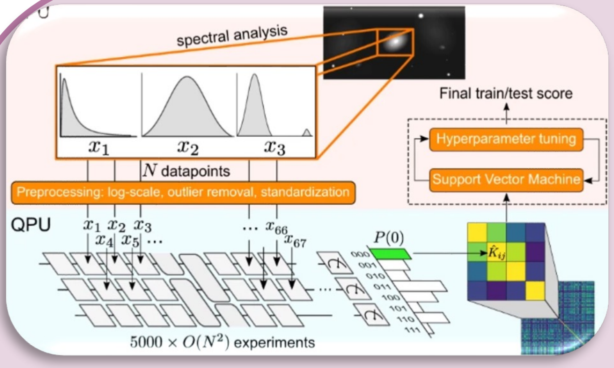
$$2^{275}$$

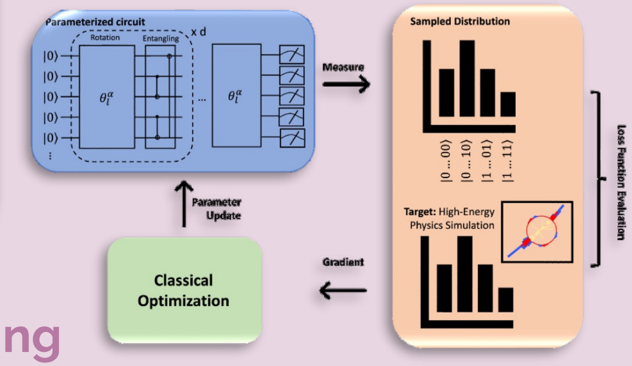
But it is also very hard! – *Andrea Delgado*



Applications in High-Energy Physics : Quantum Machine Learning

Quantum Computing Applications in High-Energy Physics



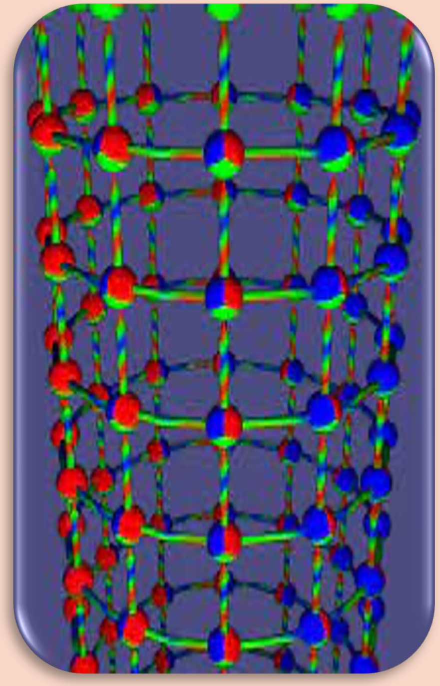


Quantum Machine Learning

- Supervised learning: Classification based on kernel methods, optimization.
- Unsupervised learning: Generative modeling, data augmentation.

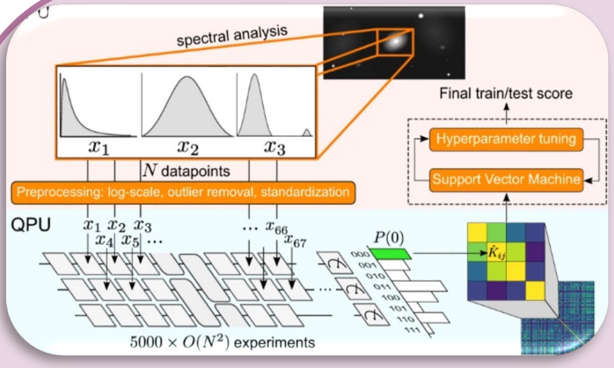
Field theory simulation

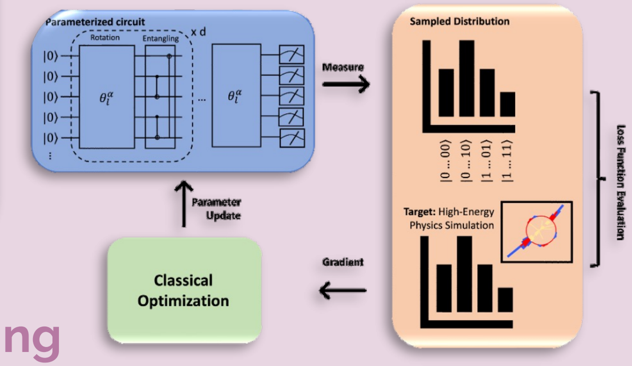
- Mapping fermionic/bosonic degrees of freedom into quantum system.
- Significant overlap with condensed matter.



Bauer, C. W., et al **Quantum Simulation for High Energy Physics,** arXiv: e-Print: 2204.03381 [quant-ph]

Quantum Computing Applications in High-Energy Physics





Quantum Machine Learning

- Supervised learning: Classification based on kernel methods, optimization.
- Unsupervised learning: Generative modeling, data augmentation.

The focus of this talk

Quantum Machine Learning

The main goal of Quantum Machine Learning (QML) is to speed things up by applying what we know from quantum computing to machine learning

Quantum Computing

- Exponentially large Hilbert space
- Entanglement
- Superposition
- Interference

Machine Learning

- Inference
- Optimization
- Fitting over a large feature/hyperparameter space

QML takes elements from classical machine learning theory, and views quantum computing from that lens

Quantum Machine Learning

The main goal of Quantum Machine Learning (QML) is to speed things up by applying what we know from quantum computing to machine learning

Quantum Computing

- Exponentially large Hilbert space
- Entanglement
- Superposition
- Interference

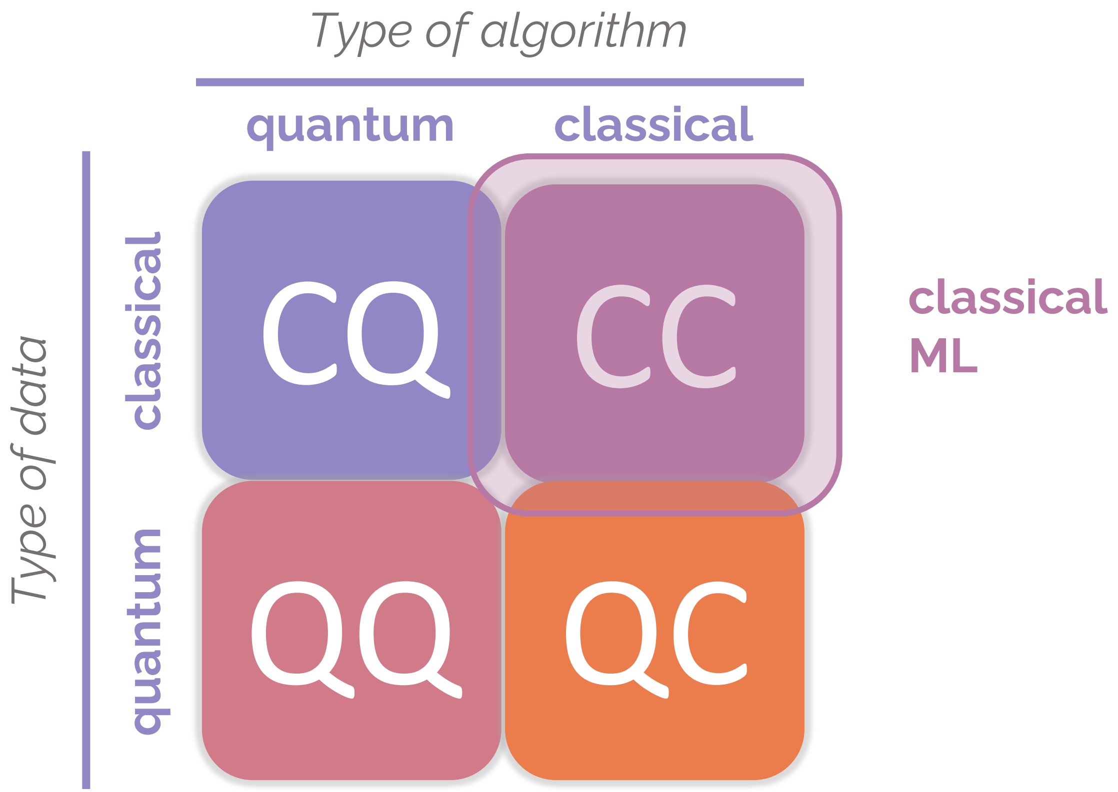
Quantum Computing ∩ Machine Learning

- Linear algebraic problems
- Kernel methods
- Optimization
- Deep quantum learning

Machine Learning

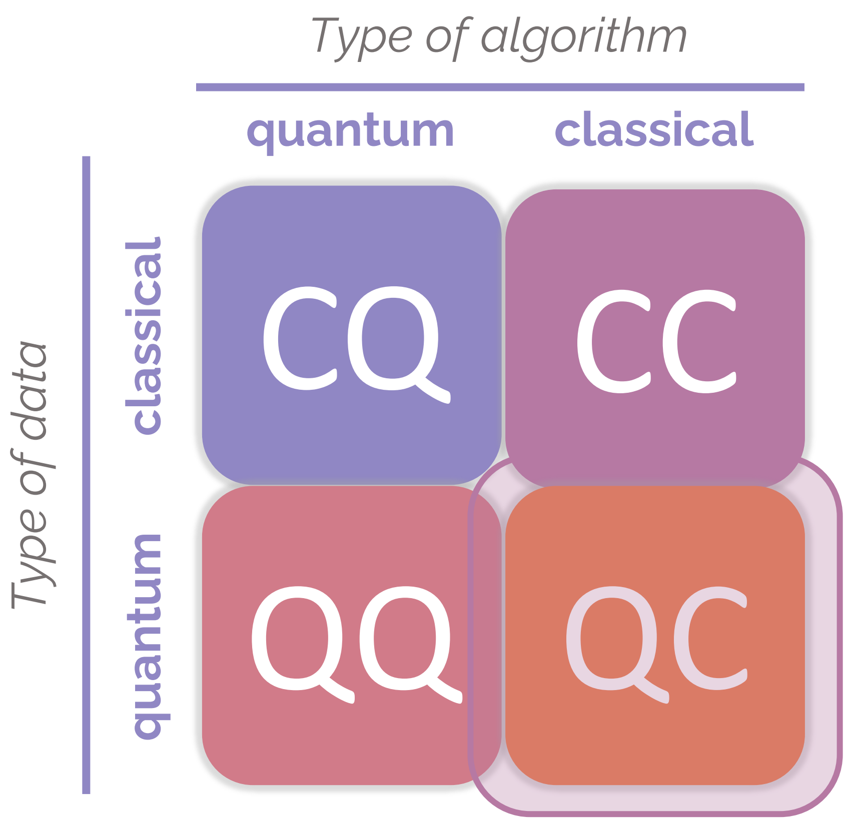
- Inference
- Optimization
- Fitting over a large feature/hyperparameter space

Quantum Machine Learning



The intersection of quantum computing and ML is rich!

Quantum Machine Learning

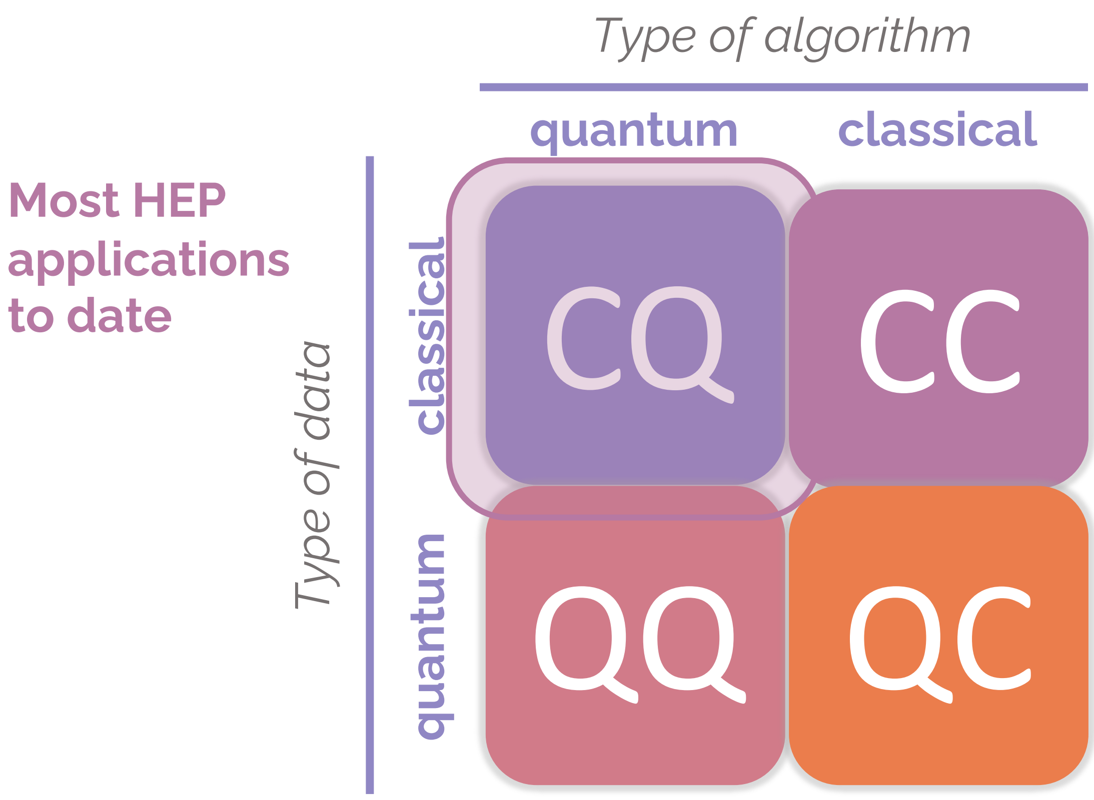


classical ML on quantum data

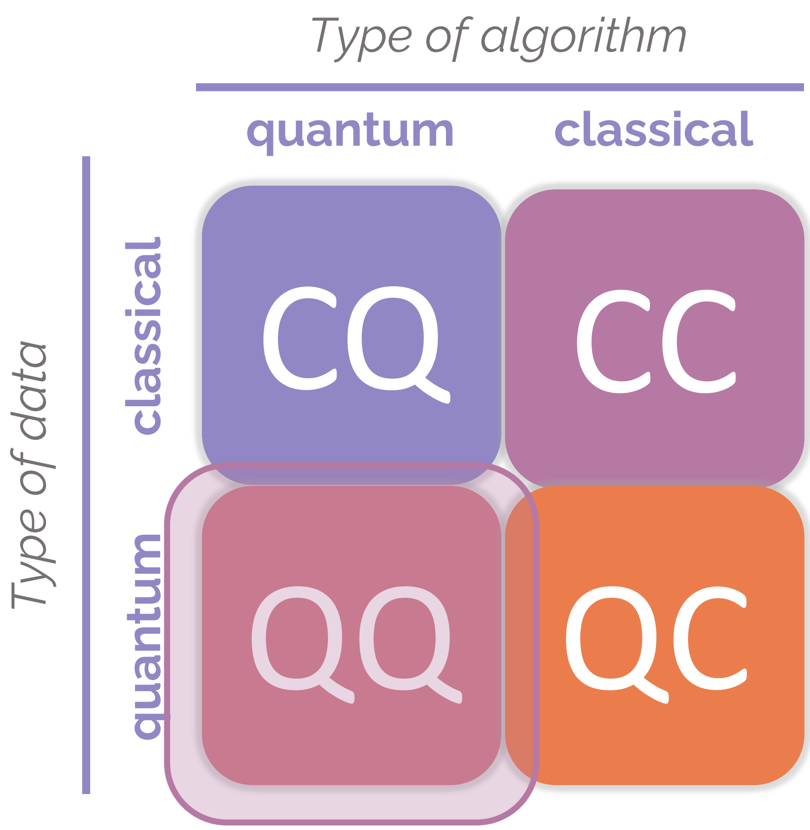
"Neural-Network Quantum States", arXiv:2204.12966

The intersection of quantum computing and ML is rich!

Quantum Machine Learning



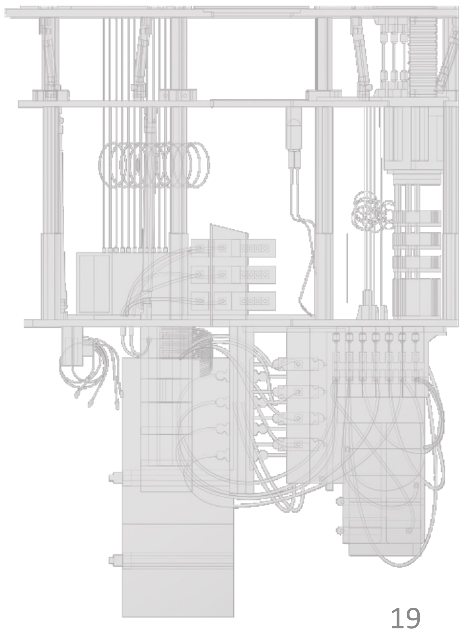
Quantum Machine Learning



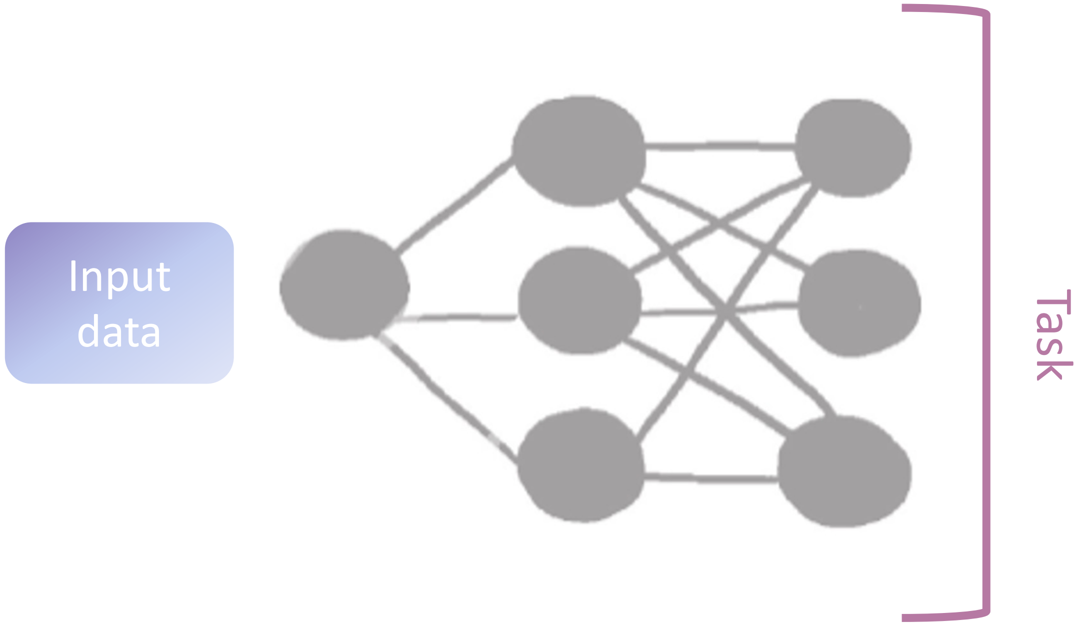
- Chemical simulation
- Quantum matter simulation
- Quantum control
- Quantum networks
- Quantum metrology

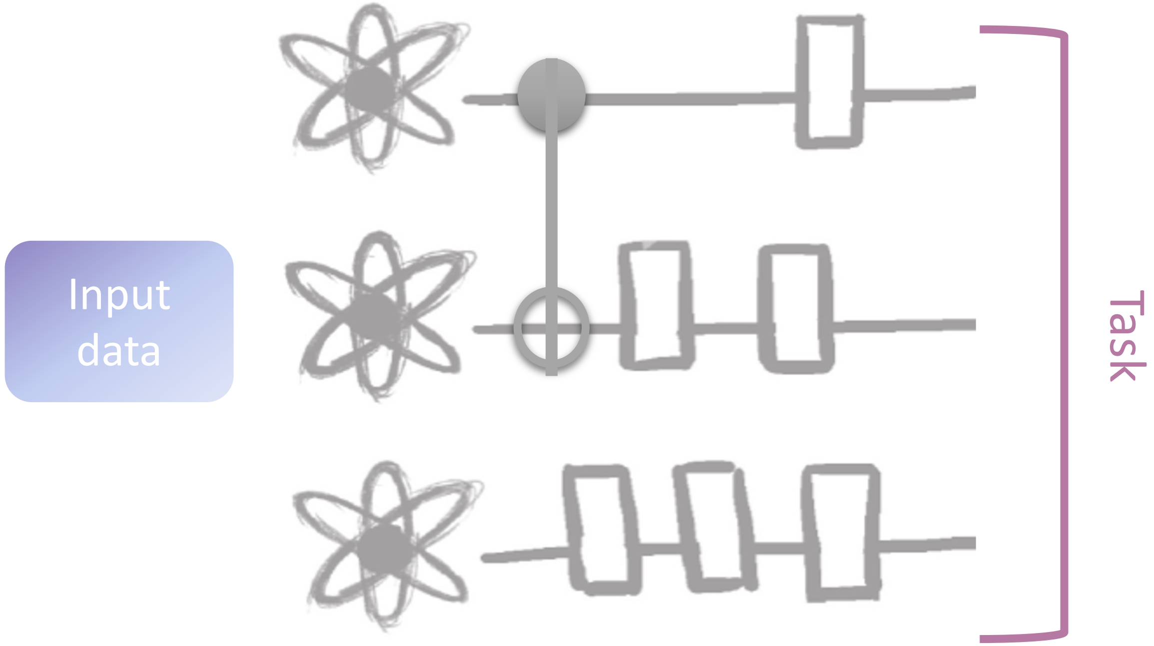
Quantum Machine Learning in the NISQ Era

- ★ Motivated by access to **cloud-based** processors and commercial applications.
- ★ Developed for deployment on **Noisy Intermediate-Scale Quantum (NISQ)** devices.
    - Few qubits,
    - Noisy,
    - Low gate fidelity – limits the number of operations that can be executed.
- ★ Applications in **Quantum Machine Learning (QML)** spurred by the release of Xanadu's PennyLane / Google's Tensorflow.
- ★ **Co-design**:
    - *Algorithmic development/research is adapting to match the pace of hardware development.*
- ★ Hybrid frameworks to leverage benefits of both classical and quantum computing - ***variational quantum circuits***.



Parameterized Quantum Circuits as ML Models



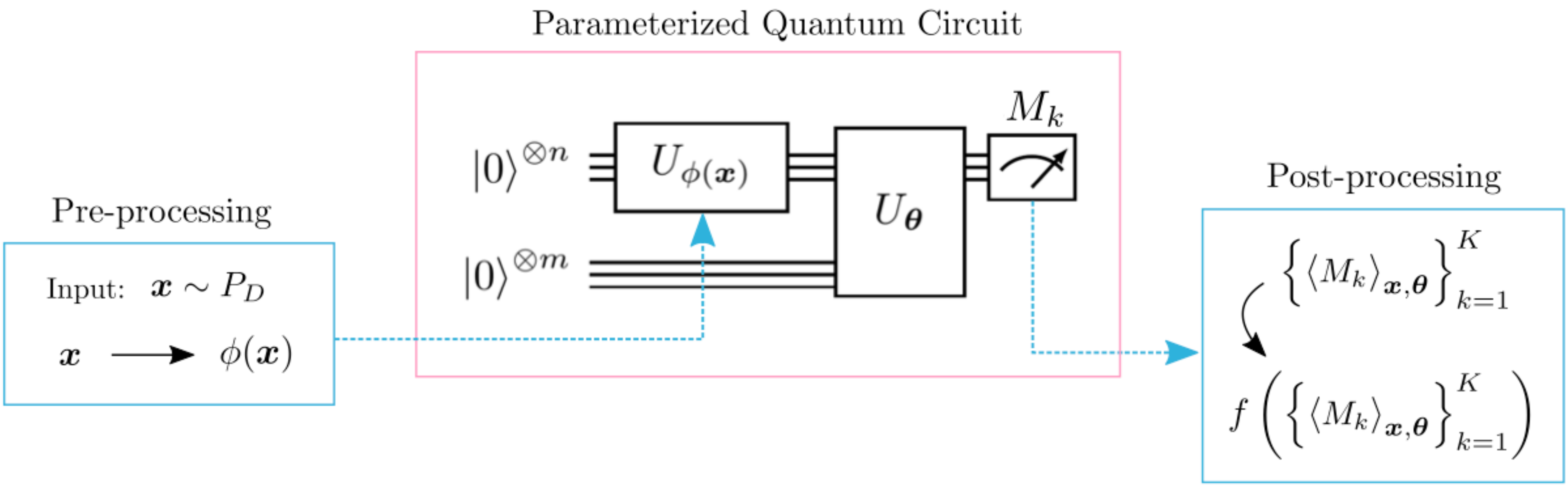


Benedetti, arXiv:1906.07682

In both cases, learning describes the process of iteratively updating the model's parameters towards a goal

Parameterized Quantum Circuits as ML Models

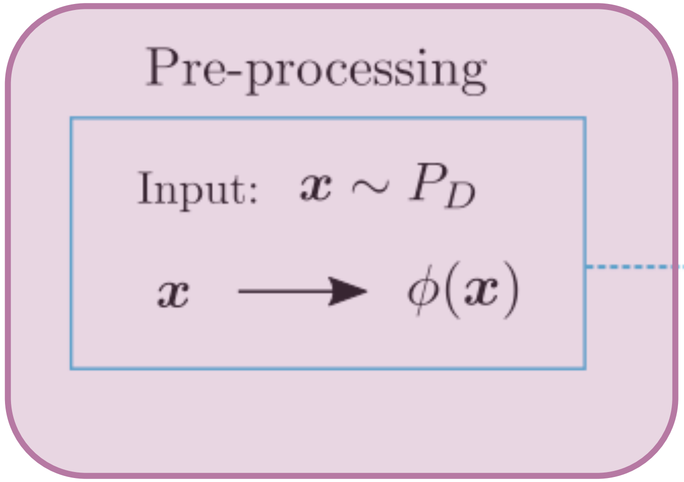
Benedetti, arXiv:1906.07682

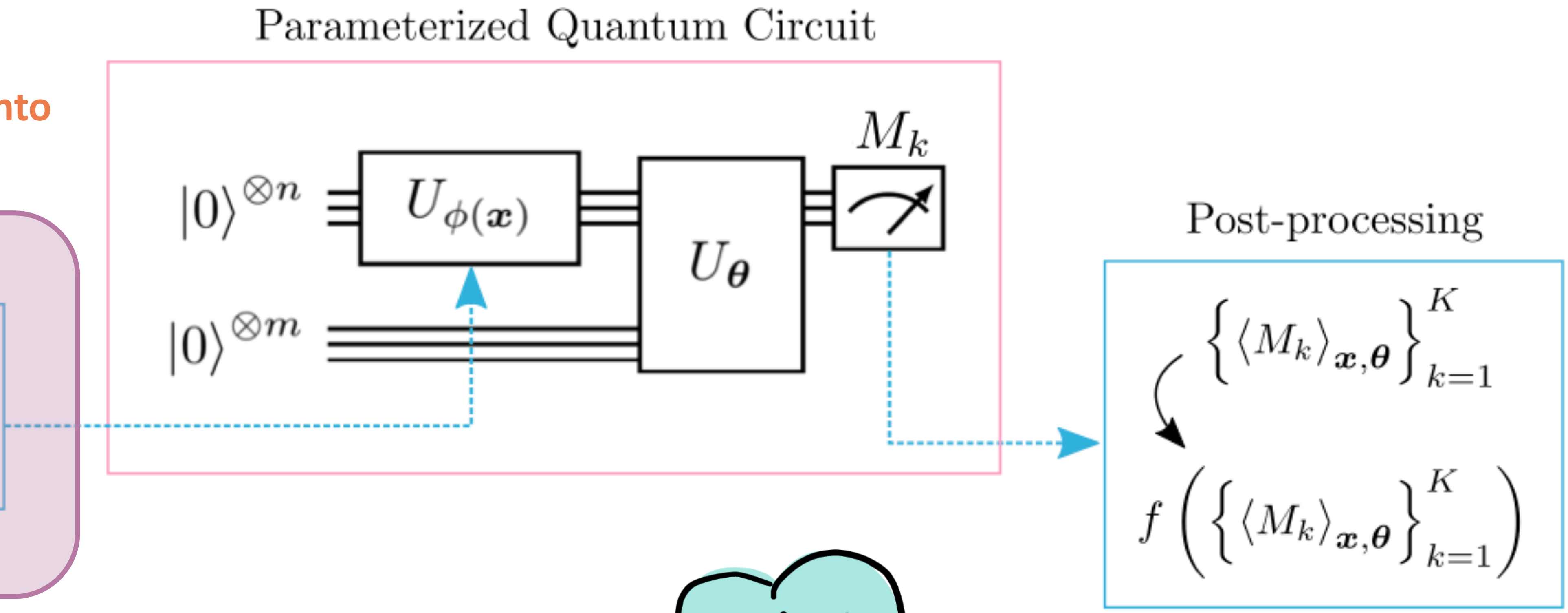


Parameterized Quantum Circuits as ML Models

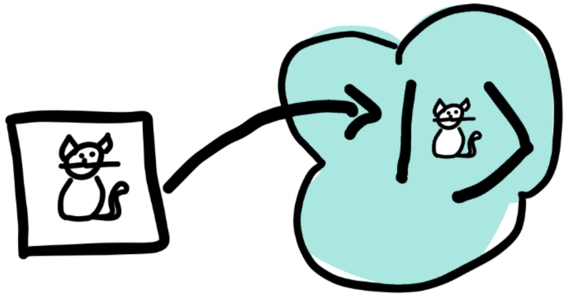
Benedetti, arXiv:1906.07682

How to encode data into a quantum state?





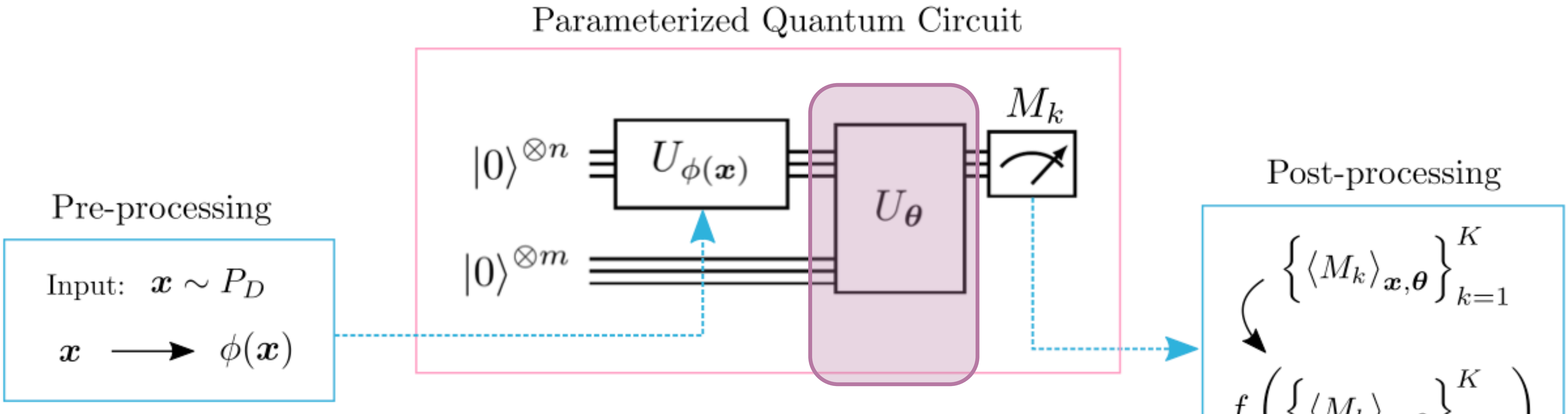
1. Start from a feature vector ***x.***
2. <u>Optional:</u> dimensionality reduction, PCA, etc.
3. Quantum embedding through a quantum feature map: *Basis embedding, amplitude embedding.*



- ★ Havlicek, et al, arXiv:1804.11326
- ★ Schuld, Killoran, arXiv:1803.07128
- ★ Lloyd, Schuld, et al, arXiv:2001.03622

Parameterized Quantum Circuits as ML Models

Benedetti, arXiv:1906.07682

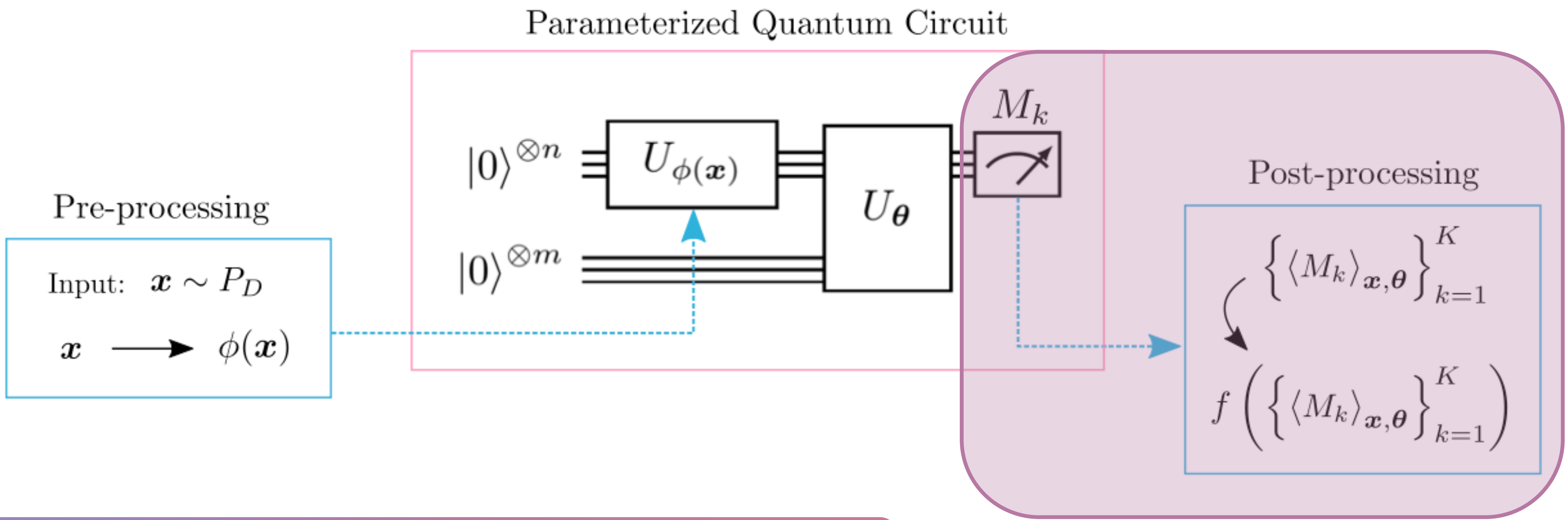


The "variational", optimizable part of the circuit.

The "guess" or trial function is the unitary U parameterized by a set of free parameters θ that will be updated during training.

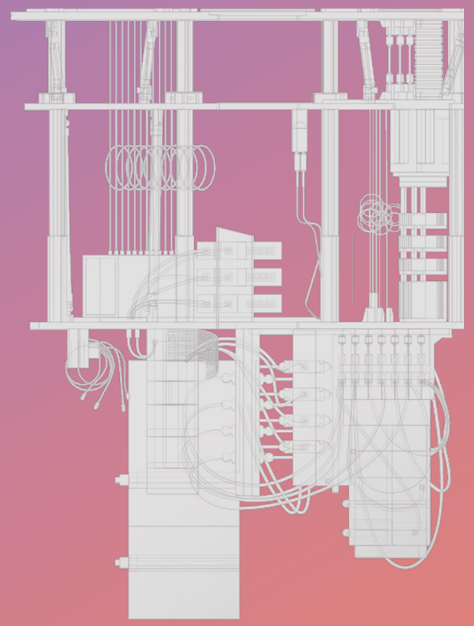
Parameterized Quantum Circuits as ML Models

Benedetti, arXiv:1906.07682



Quantum information is turned back into classical information by evaluating the expectation value of an observable, or measurement.

The measurement output is then used to construct a decision function, a probability distribution, a boundary, etc.



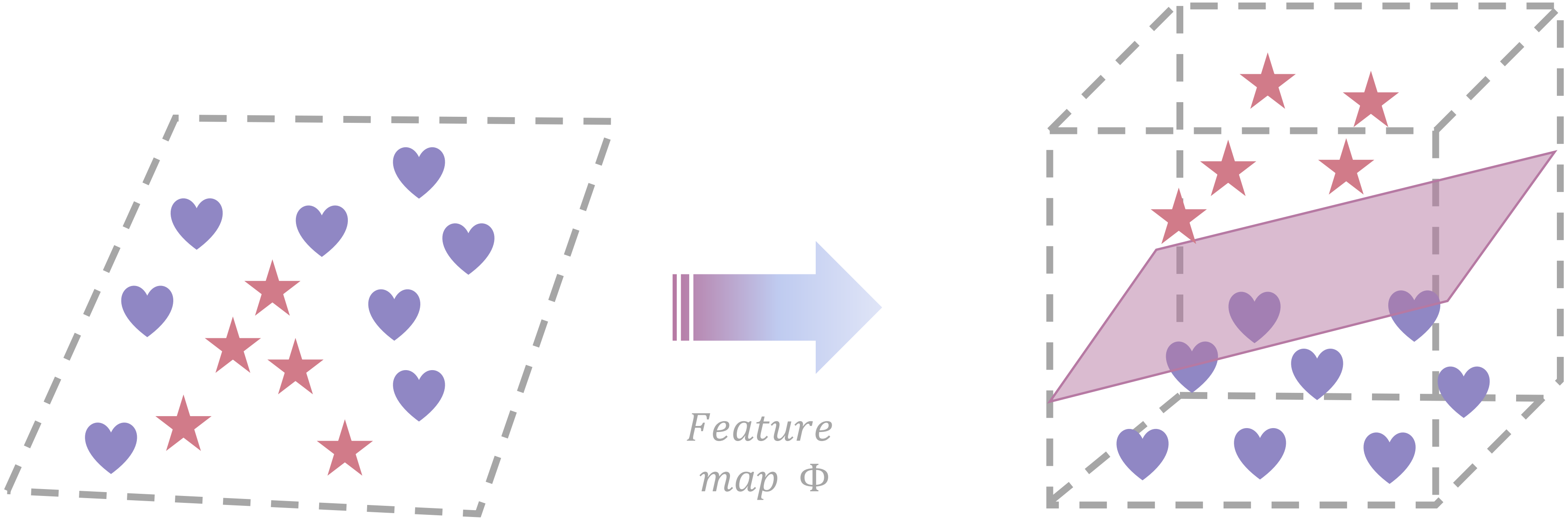
Applications

Supervised Learning with Kernel-based Quantum Models

Quantum machine learning models for supervised learning and kernel methods are based on a similar principle.

A high-level overview, for more details check references: *arXiv:2101.11020, Phys. Rev. Lett. 122, 040504 (2019), Nature. vol. 567, pp. 209-212 (2019)*

Kernel Trick



Input Space

Feature Space

Supervised Learning with Kernel-based Quantum Models

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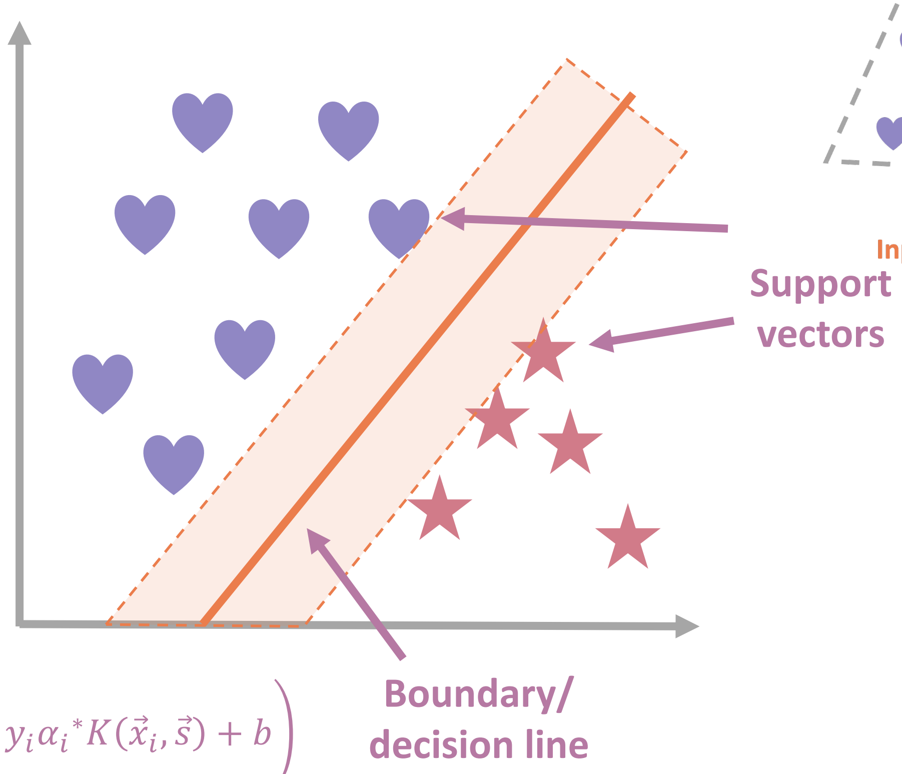
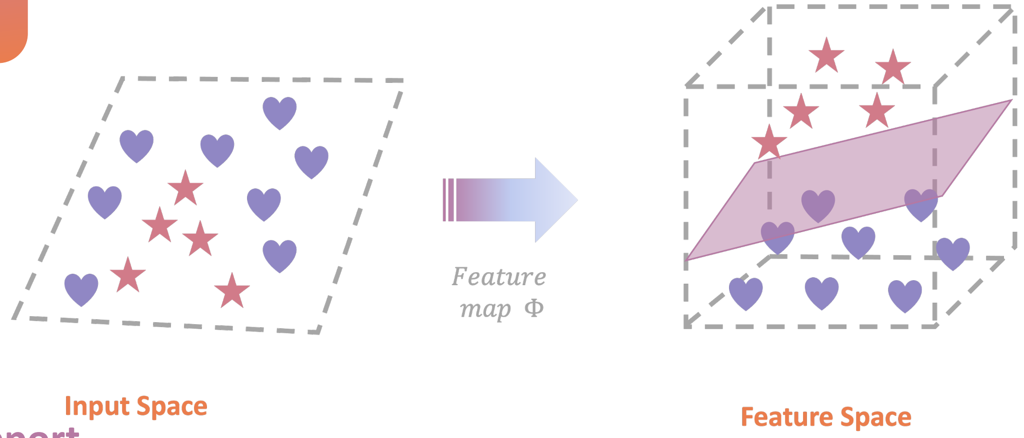
Support Vector Machine



$$\tilde{m}(\vec{s}) = sign\left(\sum_{i=1}^{t} y_i {\alpha_i}^* K(\vec{x}_i, \vec{s}) + b\right)$$



To optimize a loss function of the form

Kernel

$$L_D(\alpha) = \sum_{i=1}^{t} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{t} y_i y_j \alpha_i \alpha_j \boxed{K(\vec{x}_i, \vec{x}_j)}$$

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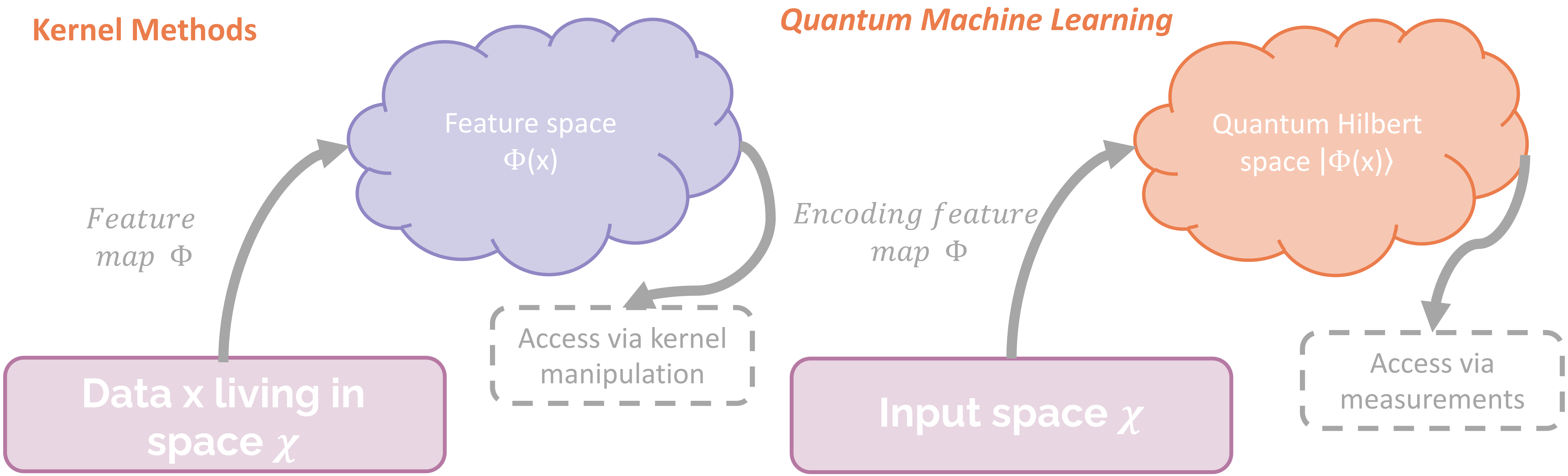

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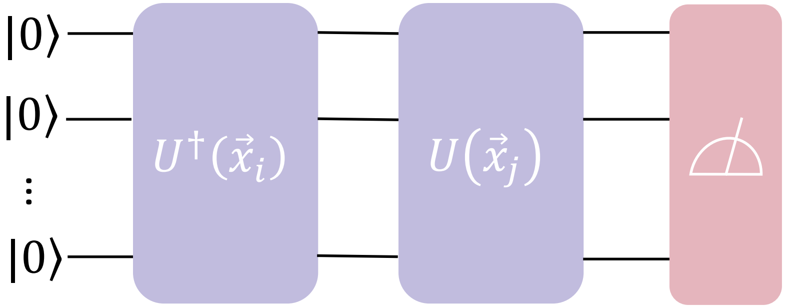
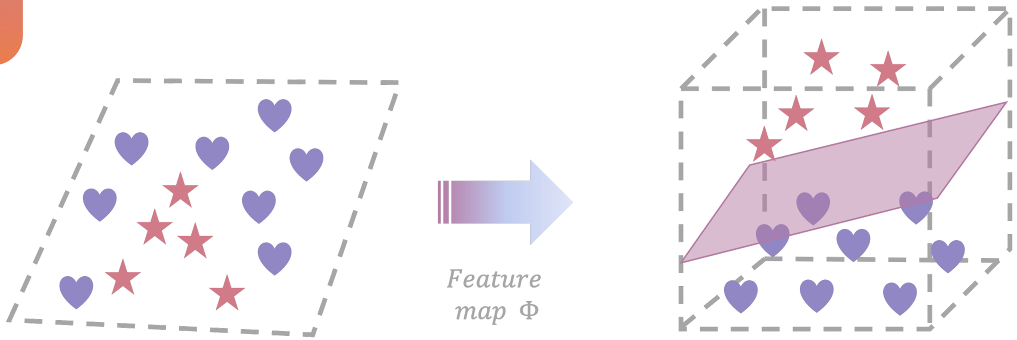
Support Vector Machine





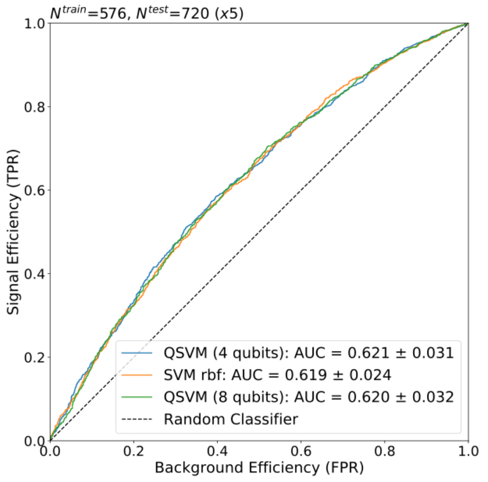
Input Space

Feature Space

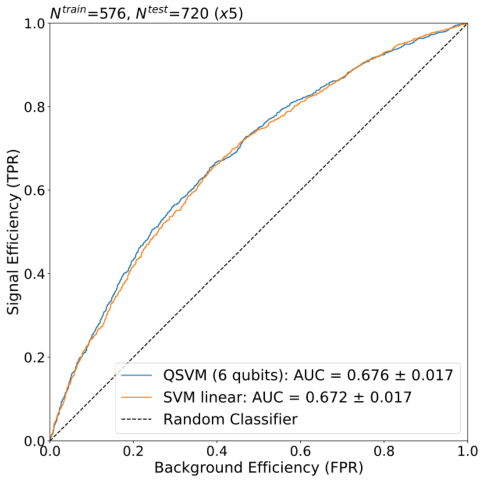
Construct a kernel matrix of the form

$$K_{ij} = \left|\langle 0|U^\dagger(\vec{x}_i)U(\vec{x}_j)|0\rangle\right|^2$$

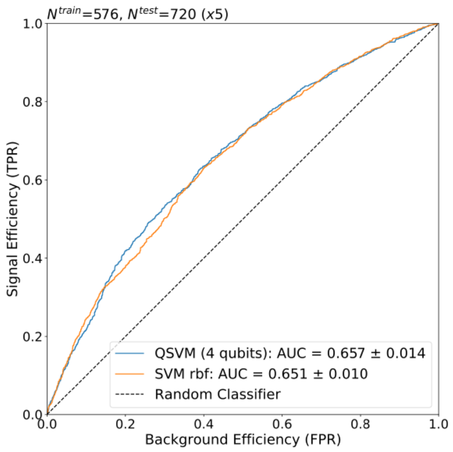
Supervised Learning with Kernel-based Quantum Models



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



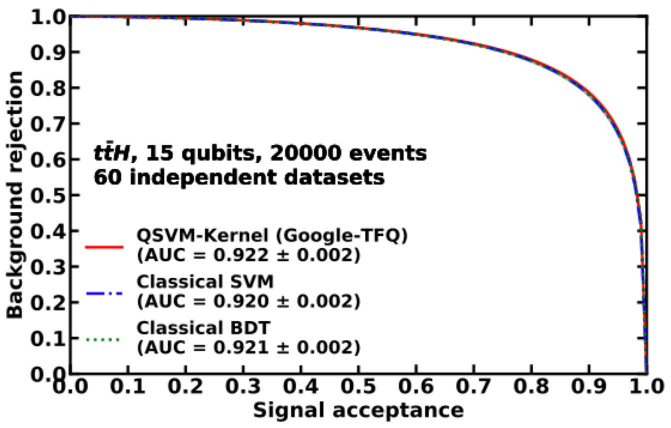
(b) Models trained on the original input features (67), discarding the 3 least informative ones (64).



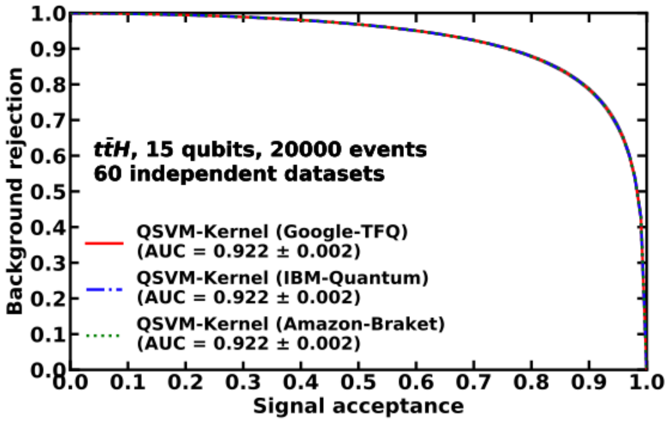
(c) Models trained on 16 selected features of the input space according to their individual AUC values.

$t\bar{t}H(b\bar{b})$ classification problem on 4,6, and 8 qubit QSVM

"Higgs analysis with quantum classifiers", Belis, Gonzalez-Castillo, et al., arXiv:2104.07692 (2021)



(a)



(b)

$t\bar{t}H$ classification problem on 20 qubit QSVM in simulation and 15 qubits in HW

"Application of Quantum Machine Learning Using the Quantum Kernel Algorithm on High-Energy Physics Analysis at the LHC", Wu, Sun, Guan, et al., arXiv:2104.05059 (2021)

Supervised Learning with Kernel-based Quantum Models

The importance of choosing a good feature map

Signal/background classification problem on 6 qubit QSVM

Table 1 Average results from 10 random dataset samples obtained by classically simulating various encoding circuits using Qiskit *statevector_simulator* with 60,000 training events and 10,000 testing events in each sample

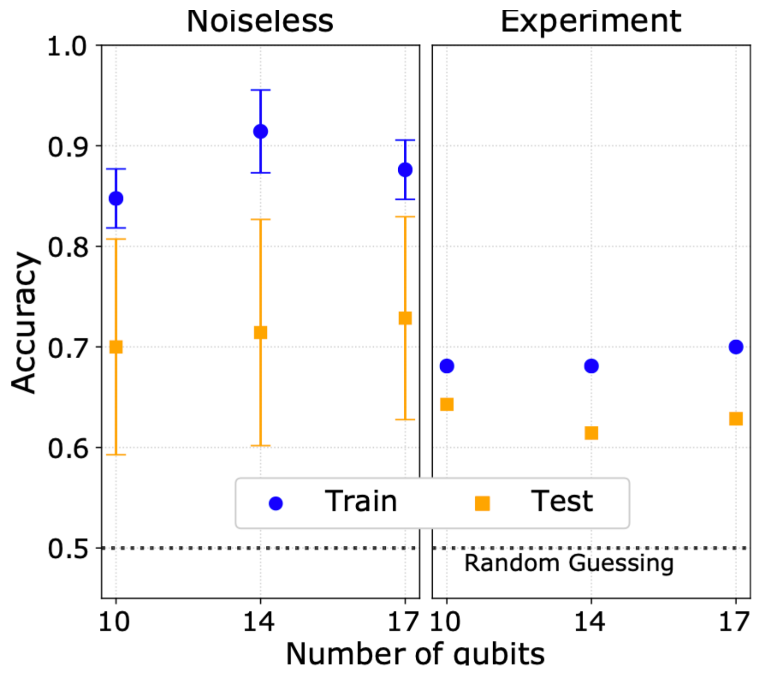
Encoding circuit	Accuracy	AUC
Combinatorial encoding	0.762	0.822
Separate particle encoding	0.776	0.835
Bloch sphere encoding	0.764	0.836
Separate particle with bloch	0.771	0.848
Classical RBF kernel SVM	0.728	0.793
XGBoost	0.590	0.621

The uncertainty on each of the mean values stated is ± 0.001

"Quantum Support Vector Machines for Continuum Suppression in B meson Decays", Heredge, Hill, Hollenberg, Sevior, Computing and Software for Big science (2021) 5:27

The effect of noise in model performance

Supernovae classification with QSVM at Google's Sycamore processor

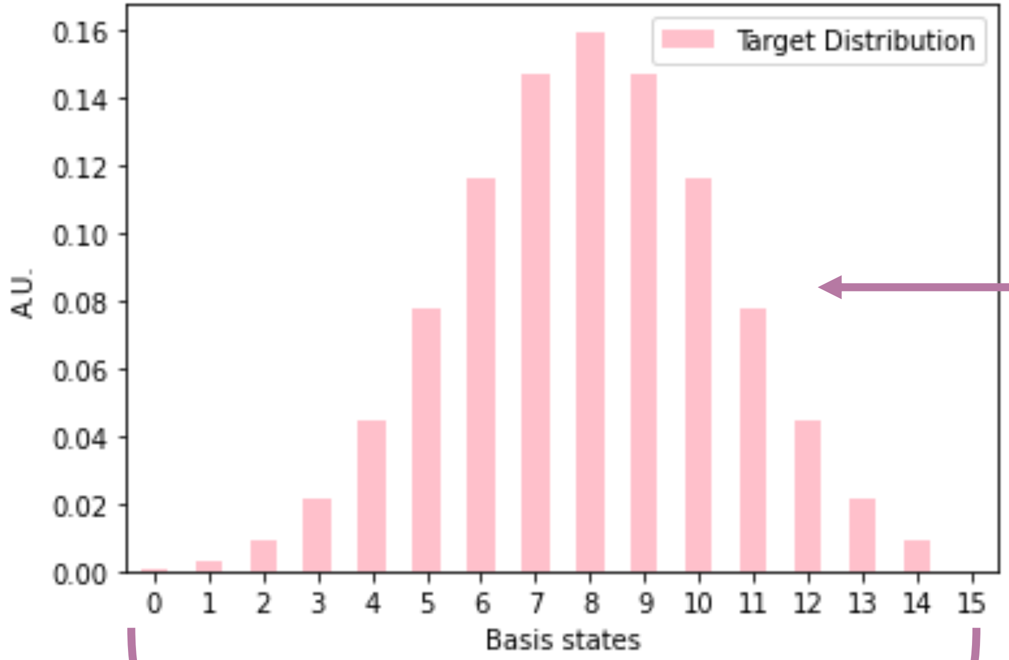


"Machine Learning of high-dimensional data on a noisy quantum processor", Peters, Caldeira, Ho, et al., npj Quantum Information (2021) 7:161

Unsupervised Generative Modeling

Quantum Circuit Born Machines are generative models which represent the probability distribution of a classical dataset as quantum pure states

A high-level overview, for more details check references: *Phys. Rev. A 98, 062324 (2018), arXiv:2203.03578*



Discretized Gaussian probability distribution over $2^{n_{qubits}}$ basis states or bins.

$2^{n_{qubits}}$ basis states or bins, i.e., 0000, 0001, 0010, etc.

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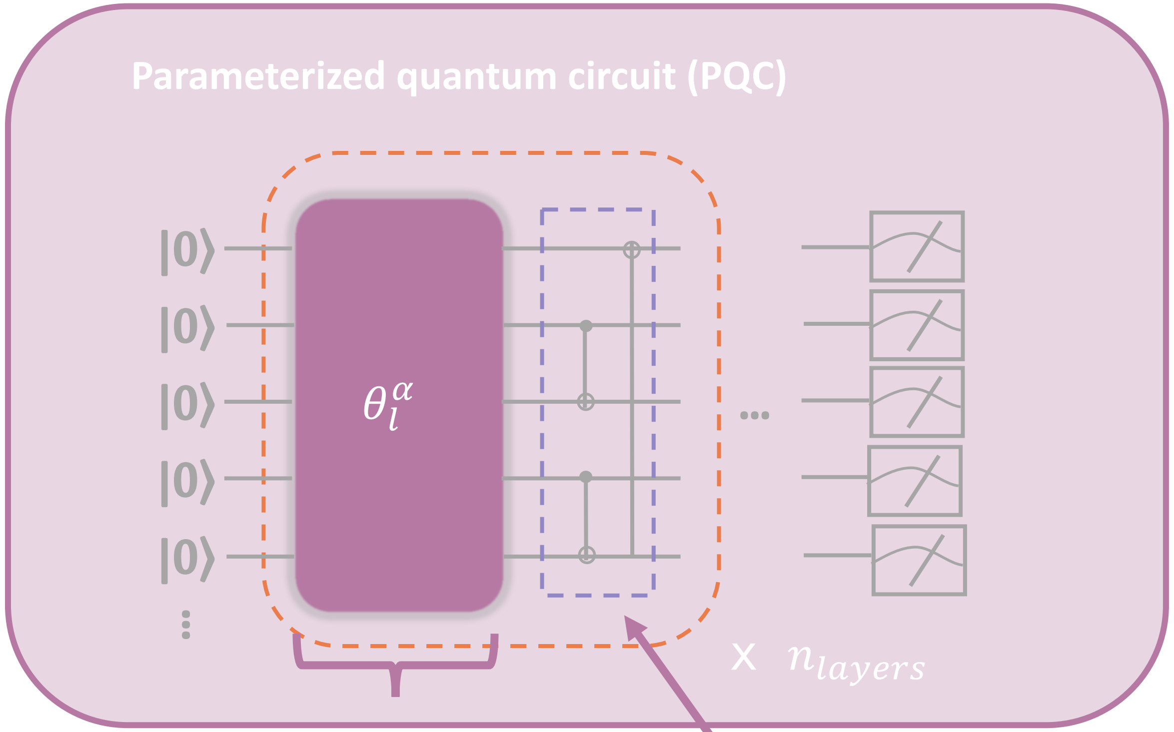

A PQC consists of layers or blocks of rotational and entangling gates that can be repeated to maximize the circuit's expressibility.

Block of rotation gates, with tunable parameters

Block of entangling gates

Discussion on smart Ansatz choices in a few slides ☺

Unsupervised Generative Modeling

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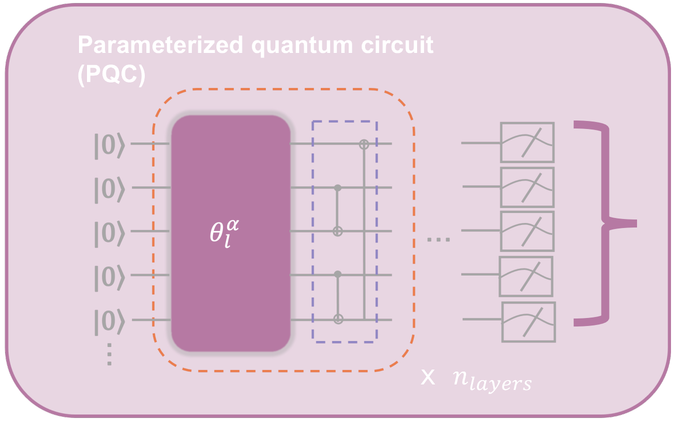
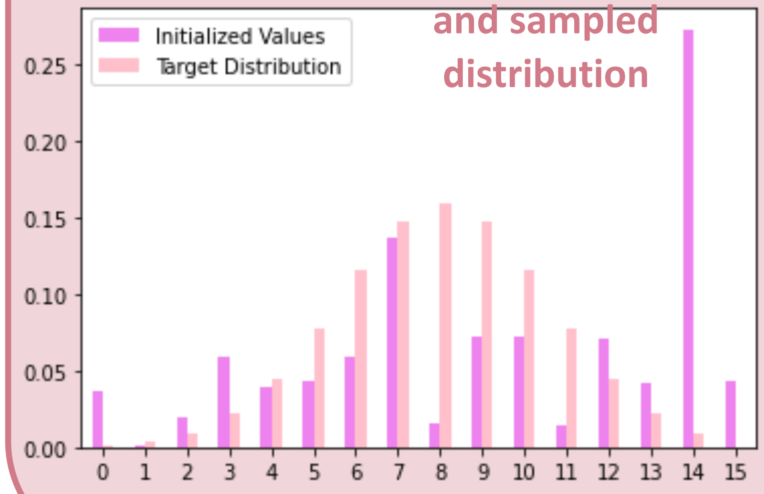


Measurement

Evaluate loss function on target and sampled distribution



Parameter update

Classical Optimization

Gradient-based optimization

Unsupervised Generative Modeling

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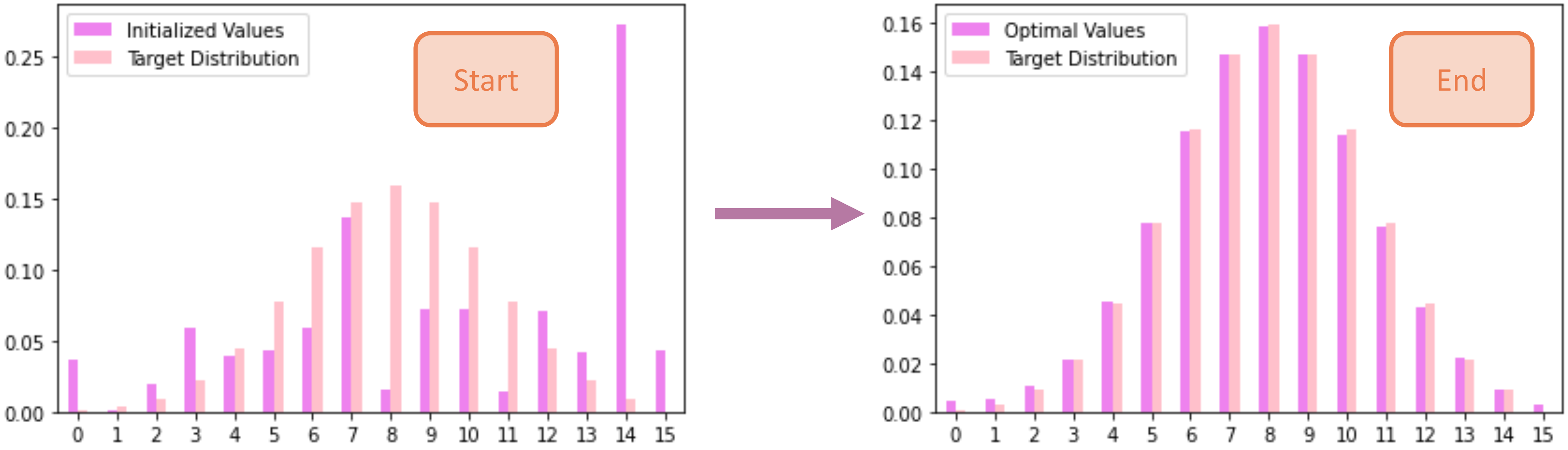
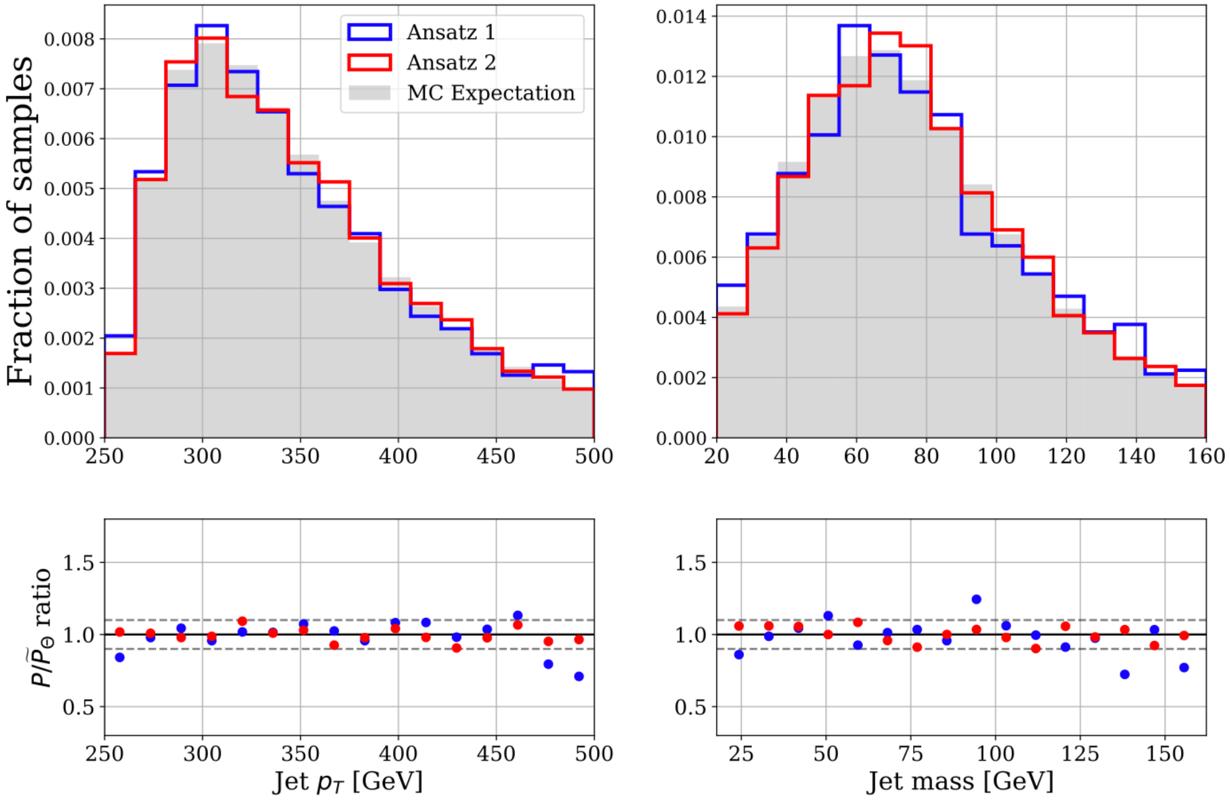


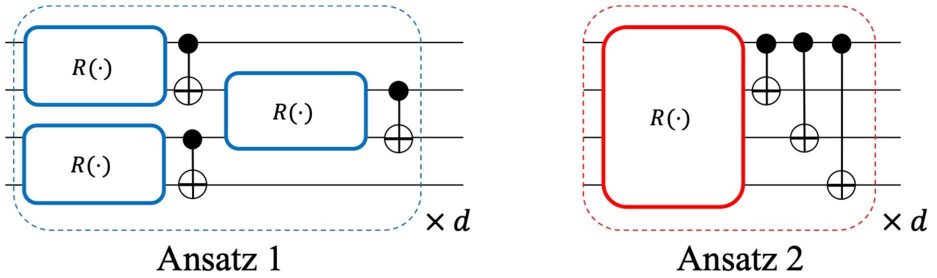
QCBM trained on 4 qubits using cosine distance metric optimized using gradient-based optimizer (Adam). Hyperparameters: learning rate = 0.1, number of steps = 100 , 8192 shots.

Unsupervised Generative Modeling

Can QCBM's learn joint distributions?

Yes!





(a) Monte Carlo (Ground Truth)

	p_T	mass
p_T	-	0.2
mass	0.2	-

(b) Ansatz 1

	p_T		mass	
	$\vert 0\rangle^{\otimes 8}$	$\vert \Phi^+\rangle^{\otimes 4}$	$\vert 0\rangle^{\otimes 8}$	$\vert \Phi^+\rangle^{\otimes 4}$
p_T	-		0.19	0.12
mass	0.19	0.12	-	

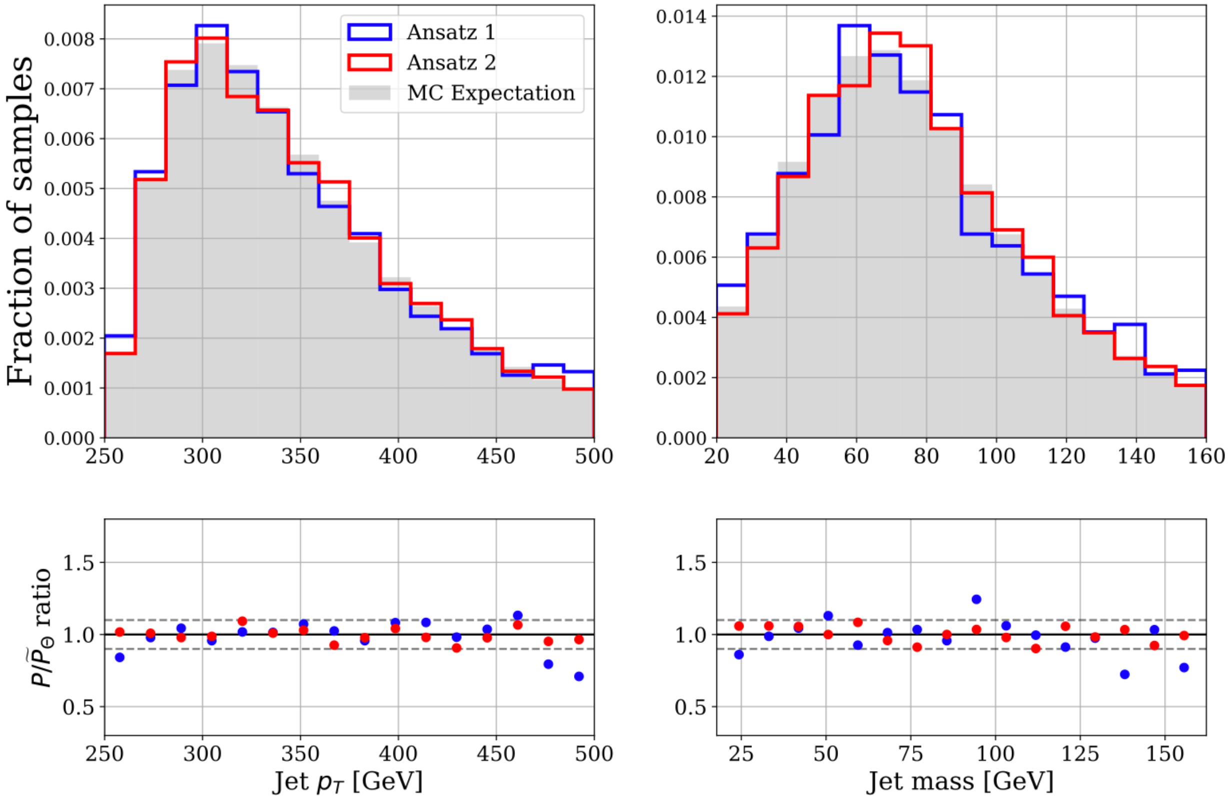
(c) Ansatz 2

	p_T		mass	
	$\vert 0\rangle^{\otimes 8}$	$\vert \Phi^+\rangle^{\otimes 4}$	$\vert 0\rangle^{\otimes 8}$	$\vert \Phi^+\rangle^{\otimes 4}$
p_T	-		-1.0e-3	-9.1e-3
mass	-1.0e-3	-9.1e-3	-	

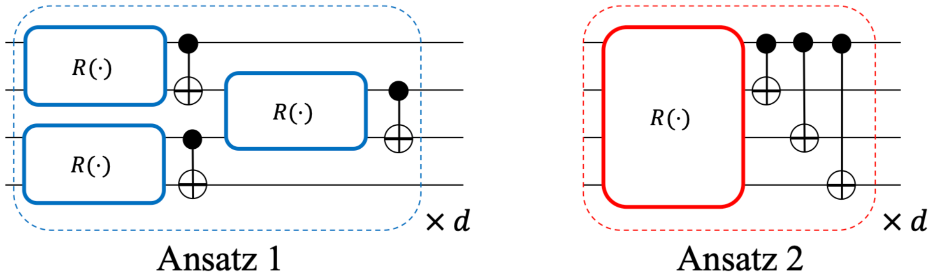
Delgado, A., Hamilton, K. E., "Unsupervised Quantum Circuit Learning in High-Energy Physics" PhysRevD 106, 096006

Unsupervised Generative Modeling

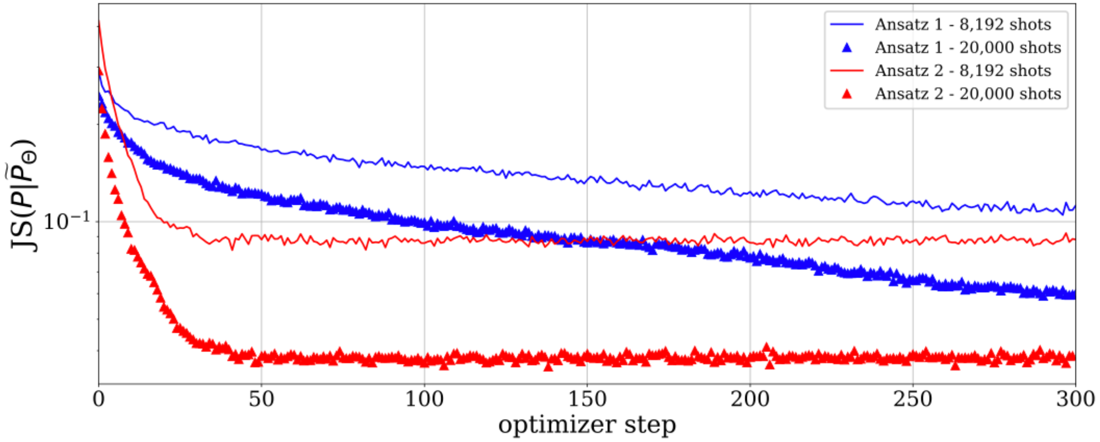
Can QCBM's learn joint distributions?



Delgado, A., Hamilton, K. E., "Unsupervised Quantum Circuit Learning in High-Energy Physics" PhysRevD 106, 096006

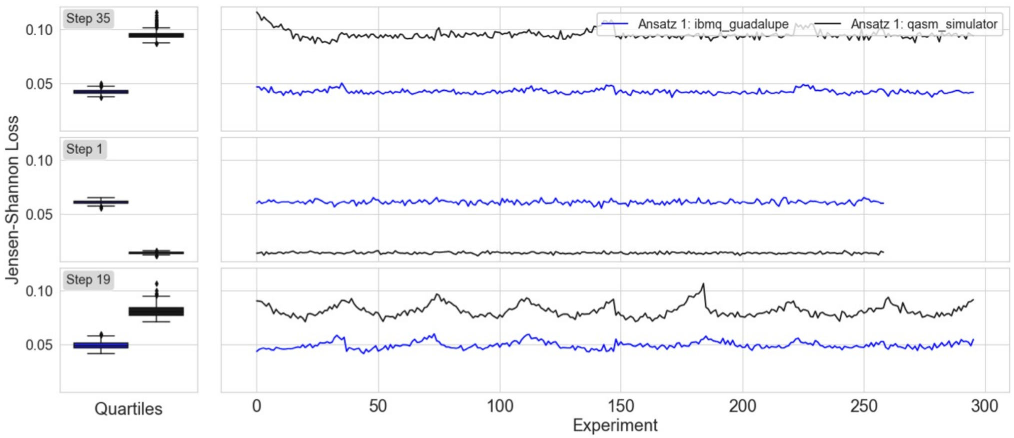


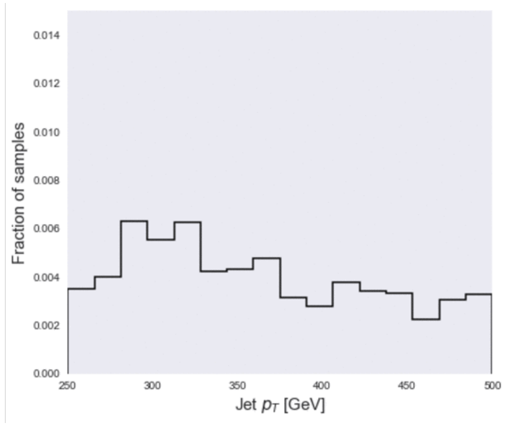
The effect of number of shots in training

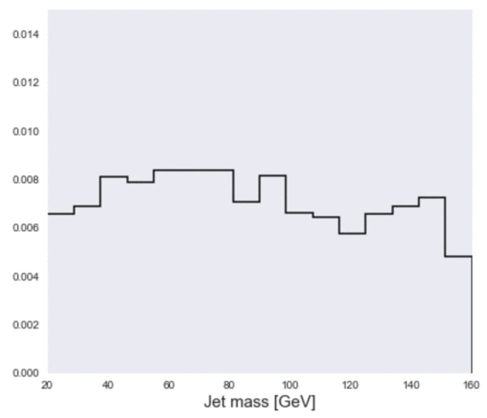


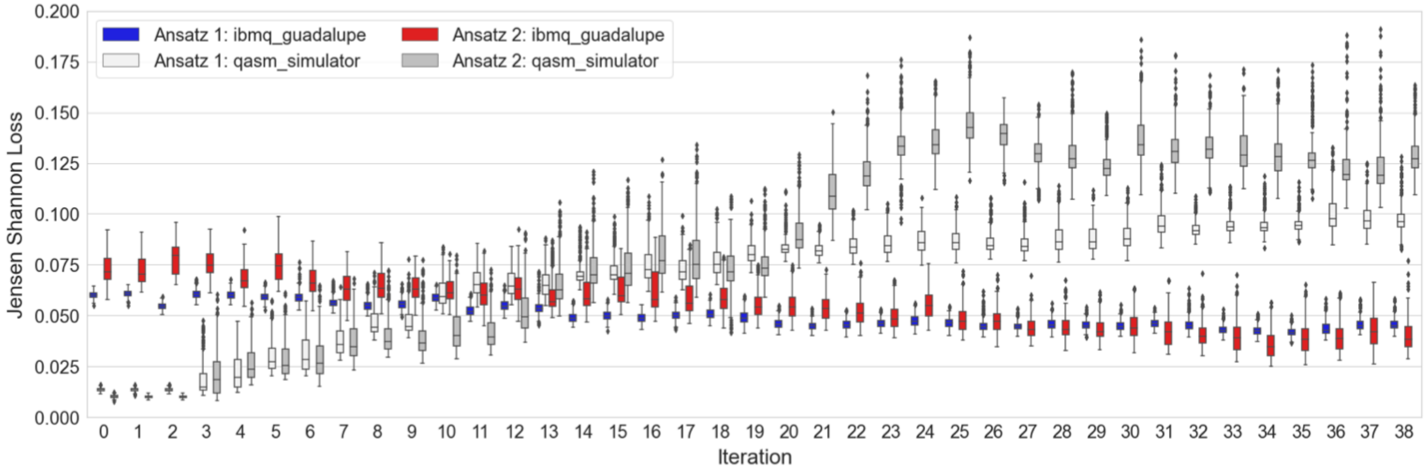
Unsupervised Generative Modeling

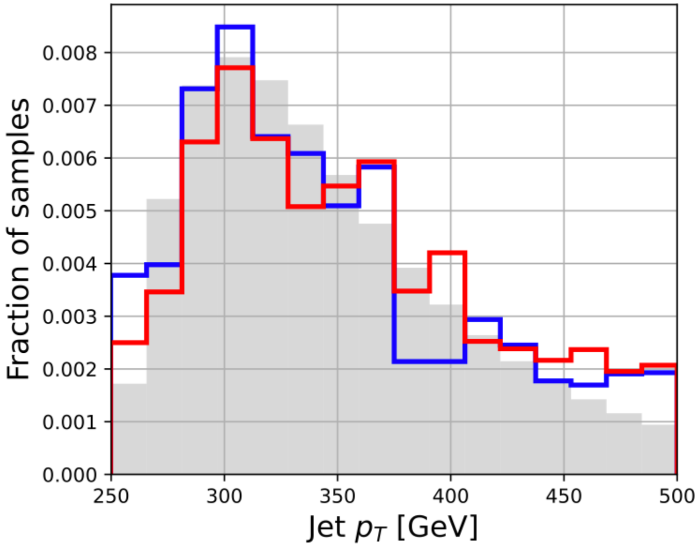
What about hardware noise?

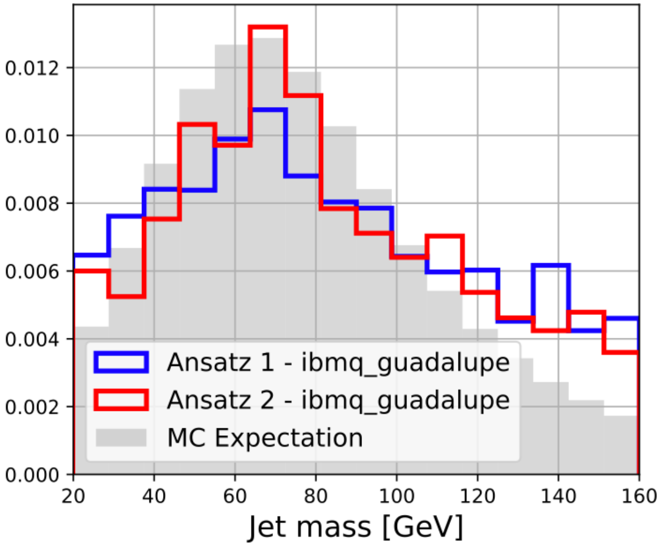




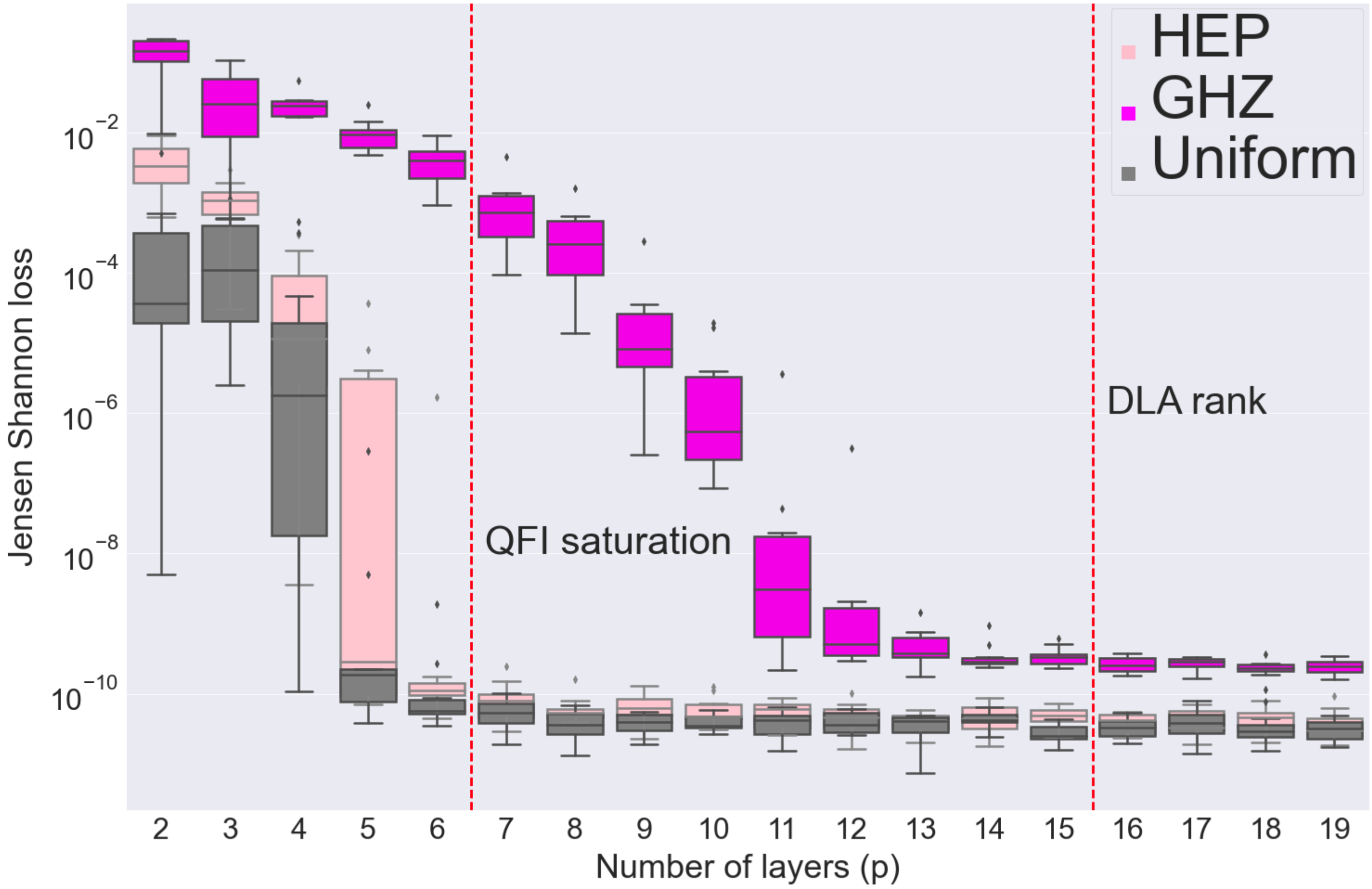








Currently working on…

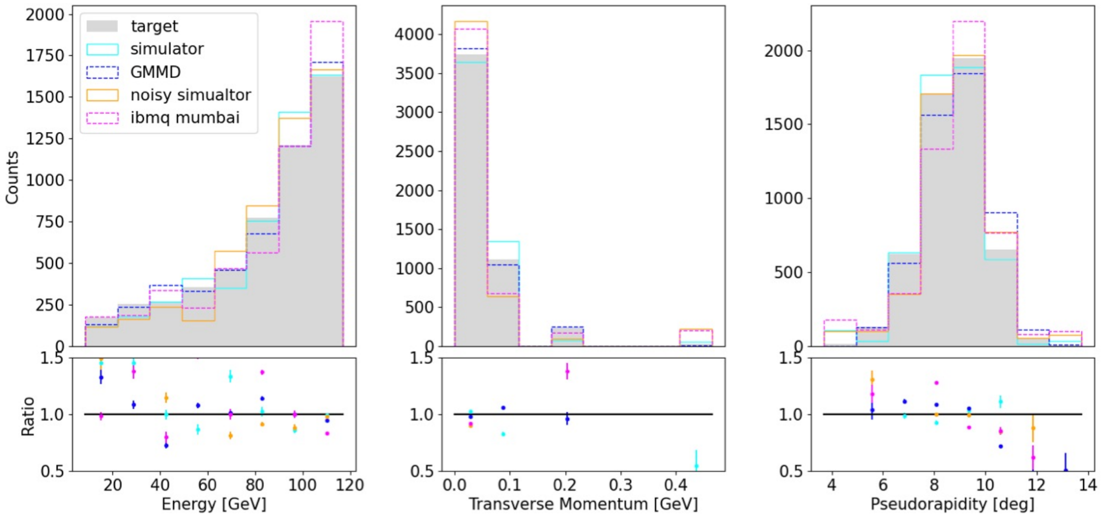


Model capacity in terms of parameter dimension D

$$D = 2^{n+1} - 2$$

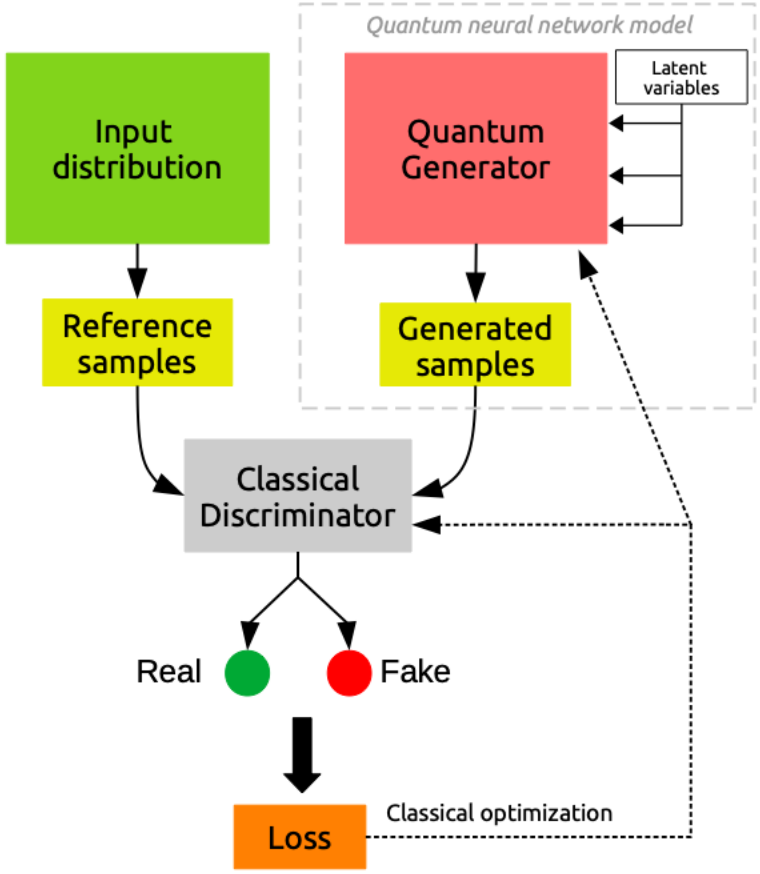
Define regions of over/underparameterization?

Also check out:



(a) Energy (b) Transverse momentum (c) pseudorapidity

”Conditional Born machine for Monte Carlo events generation”, Kiss, O., Grossi, M., Kajomovitz, E., Vallecorsa, S., arXiv:2205.07674

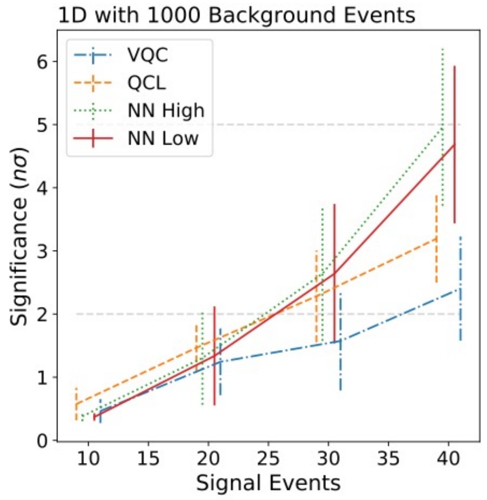


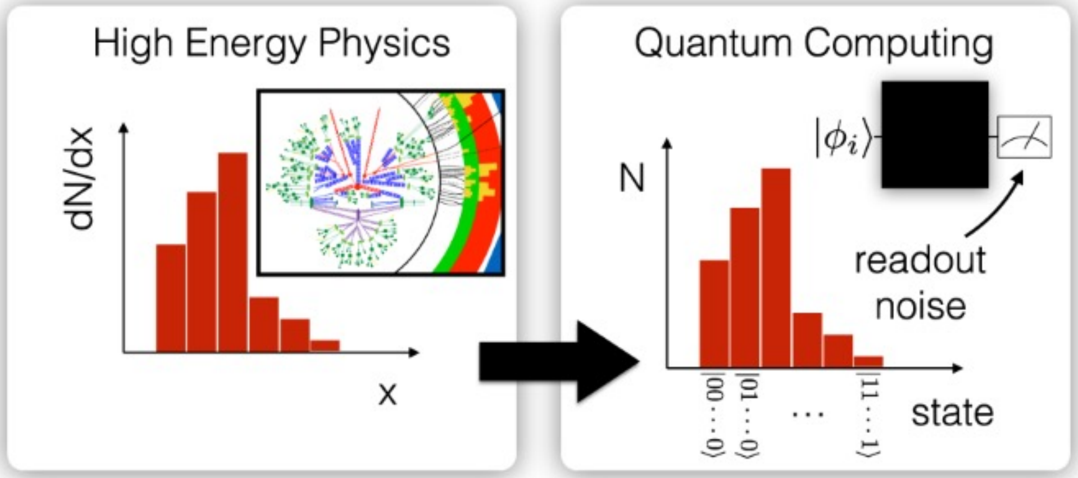
”Style-based quantum generative adversarial networks for Monte Carlo events”, Bravo-Prieto, C., Baglio, J., Ce, M., Francis, A., Grabowska, D., Carrazza, S., arXiv: 2110.06933

QML Applications for Data Analysis in HEP: Lessons Learned

- ★ On training from few data…
  - ★ Low statistics vs significance
- ★ QML is not going to solve big data problems.
  - ★ Encoding of classical information cancels out any potential quantum advantage.
  - ★ Can we harness the intrinsically quantum/physical structure of our data?
- ★ What can HEP do for QML?
  - ★ i.e., unfolding quantum computer readout noise.

Alvi, S. , Bauer, C., Nachman, B., arXiv:2206.08397





Nachman, B., et al, npj Quantum Information 6, 84(2020)

But also… can we re-evaluate our current experiments in BSM searches?

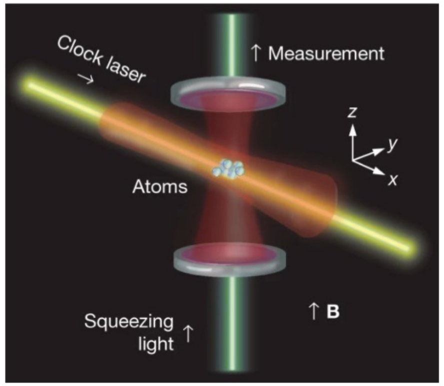
Recent developments in **quantum sensing** has inspired novel ideas for dark matter detection through quantum-enhanced techniques.

- Quantum sensors are able to detect very small changes in motion, electric and magnetic fields.

★Open questions:

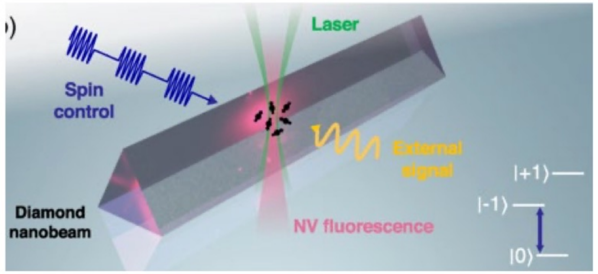
- Could they complement BSM searches at large-scale facilities such as the LHC?
- Can we couple QML algorithms to these devices?

entanglement-enhanced atomic sensors



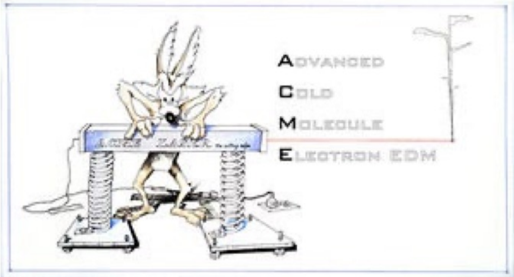
[Nature **588**, 414 (2020)]
[arXiv:2106.03754 (2021)]

NV centers in diamond



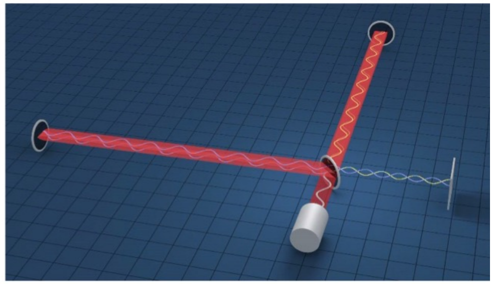
[PRX **10**, 031003 (2020)]

precisions measurements with molecules



[*Science* **343**, 269 (2013)]
[*Nature* **562**, 355 (2018)]

interferometry

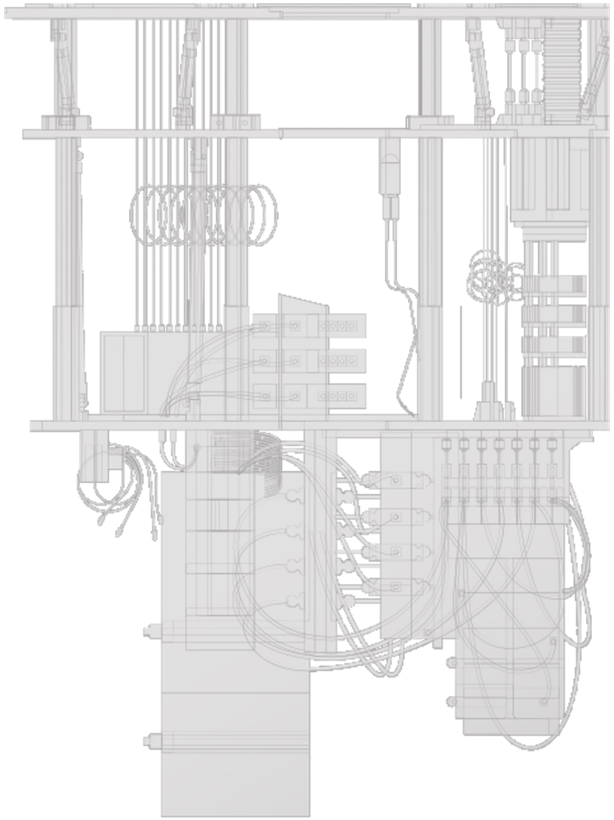


[Phys. Rev. Lett. **123**, 231107 (2019)]
[Phys. Rev. Lett. **124**, 171102 (2020)]

quantum sensing review:
[*Rev. Mod. Phys.* **89**, 035002 (2017)]

Summary

- Promising applications in HEP.
  - Finding complex correlations in data.
  - As a data augmentation tool.
  - As input models for other quantum algorithms.
  - To complement quantum-enhanced searches for BSM physics – i.e. quantum sensor networks.
- Continuous variable QML applications continue unexplored.
- Applications to data analysis outside QML exist.
- Today I only featured some applications, most of them based on discrete variable QC, targeted to IBM devices, but there are many more!
  - Delgado, A., Hamilton, K. E., Date, P., et al, ***"Quantum Computing for Data Analysis in High-Energy Physics"***, arXiv ePrint:2203.08805 [physics.data-an]



Submit your work to IEEE Quantum Week (QCE23)!

About IEEE Quantum Week

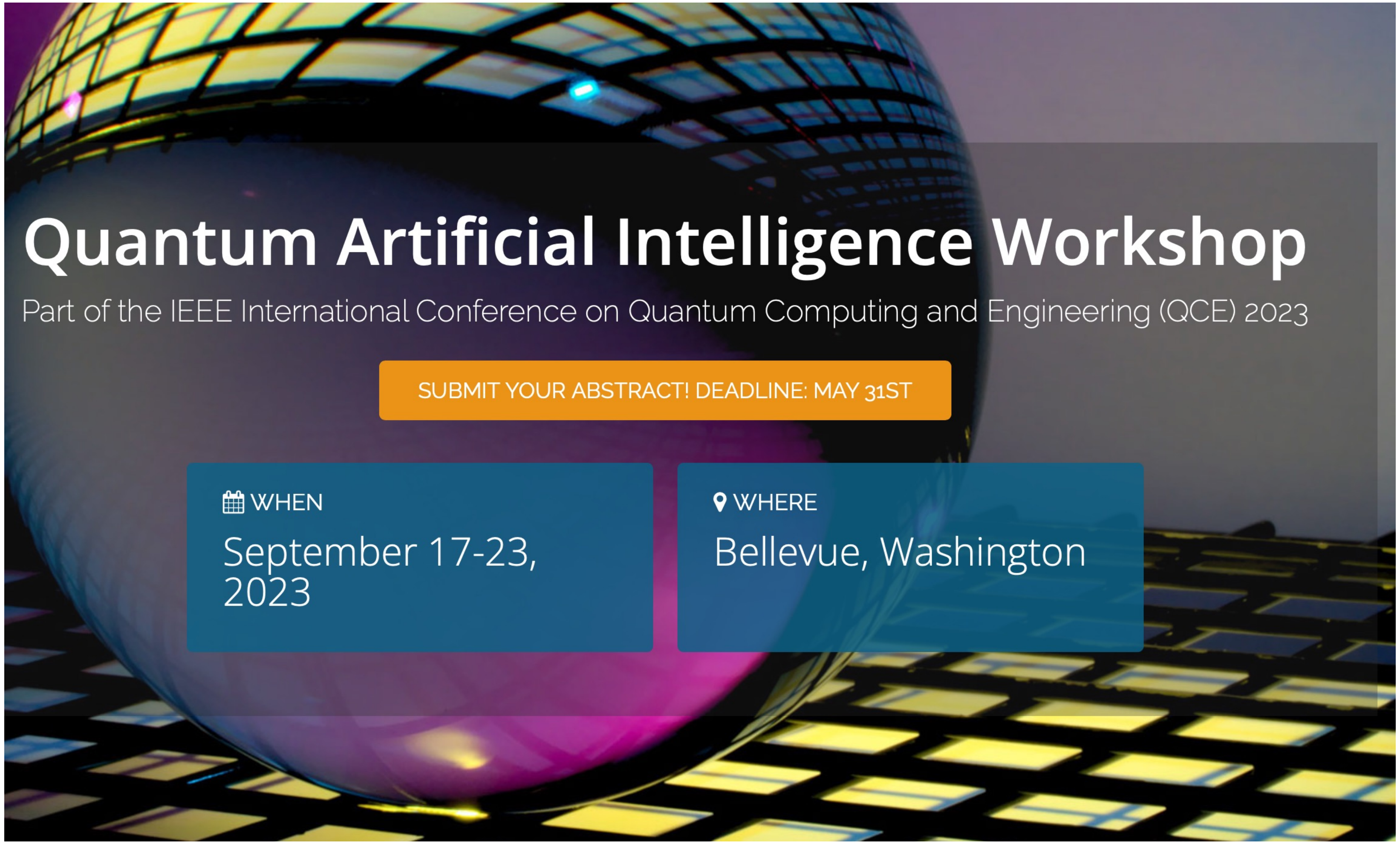
IEEE Quantum Week — the **IEEE International Conference on Quantum Computing and Engineering (QCE)** — is bridging the gap between the science of quantum computing and the development of an industry surrounding it. As such, this event brings a perspective to the quantum industry different from academic or business conferences. IEEE Quantum Week is a multidisciplinary quantum computing and engineering venue that gives attendees the unique opportunity to discuss challenges and opportunities with quantum researchers, scientists, engineers, entrepreneurs, developers, students, practitioners, educators, programmers, and newcomers.

QCE23 will be held as an **in-person event with virtual participation in Bellevue, Washington, USA** at the **Hyatt Regency Bellevue on Seattle's Eastside**. After three highly successful IEEE Quantum Week events, we are eager to develop an oustanding conference program with live exhibits, world-class keynote speakers, technical papers, community building workshops, workforce-building tutorials, stimulating panels, innovative posters, thought-provoking Birds of Feather (BoF) sessions, networking, sessions. **Attend in-person for the full conference experience! Virtual registration options are available for those who are unable to travel to Bellevue, Washington, USA.**

With your contributions and support, together we are building a wonderful premier meeting of quantum minds to help advance the fields of quantum computing and engineering. IEEE Quantum Week provides ample opportunities to network with your peers and explore partnerships with industry, government, and academia. Quantum Week 2023 aims to bring together quantum professionals, researchers, educators, entrepreneurs, champions and enthusiasts to exchange and share their experiences, challenges, research results, innovations, applications, pathways and enthusiasm on all aspects of quantum computing and engineering.

IEEE Quantum Week aims to showcase quantum research, practice, applications, education, and training including programming systems, software engineering methods & tools, hybrid quantum-classical computing, architectures & algorithms, benchmarks & performance metrics, hardware engineering, architectures, & topologies as well as many applications including simulation of chemical, physical and biological systems, optimization techniques & solutions, and quantum machine learning.

Quantum Artificial Intelligence Workshop at QCE23!



qai-workshop.ornl.gov

Thank you!

delgadoa@ornl.gov