Quantum Machine Learning Seminar

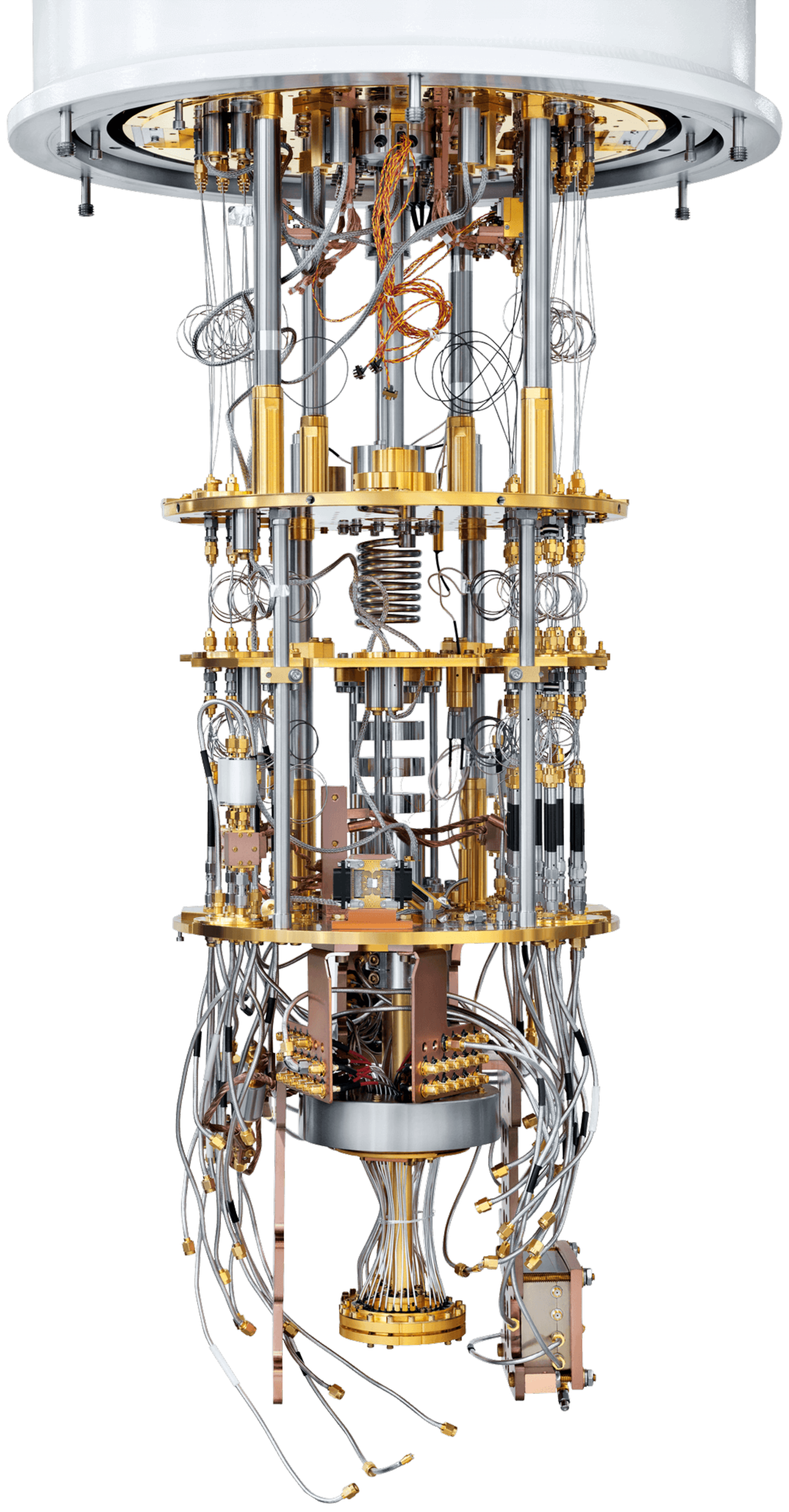
Data-Driven Quantum Mechanics

Quantum Machine Learning Seminar

Cristian E. Bello, May 10, 2025

Roadmap of the talk

1. Why, What, When Quantum Machine Learning
2. Parameterized Quantum Circuits as Machine Learning Models
3. Applications in Data Analysis
4. Barren plateaus, and how to avoid them?
5. Is Quantum Advantage the Right Goal for QML.



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.

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

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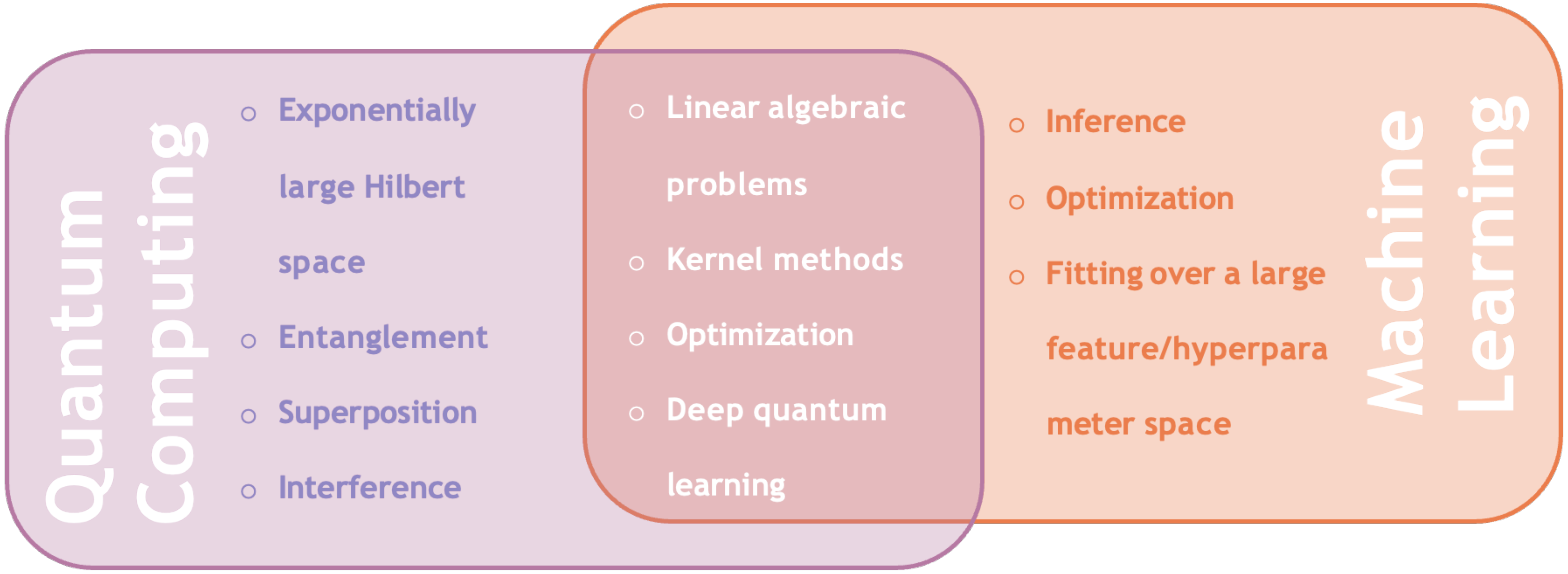
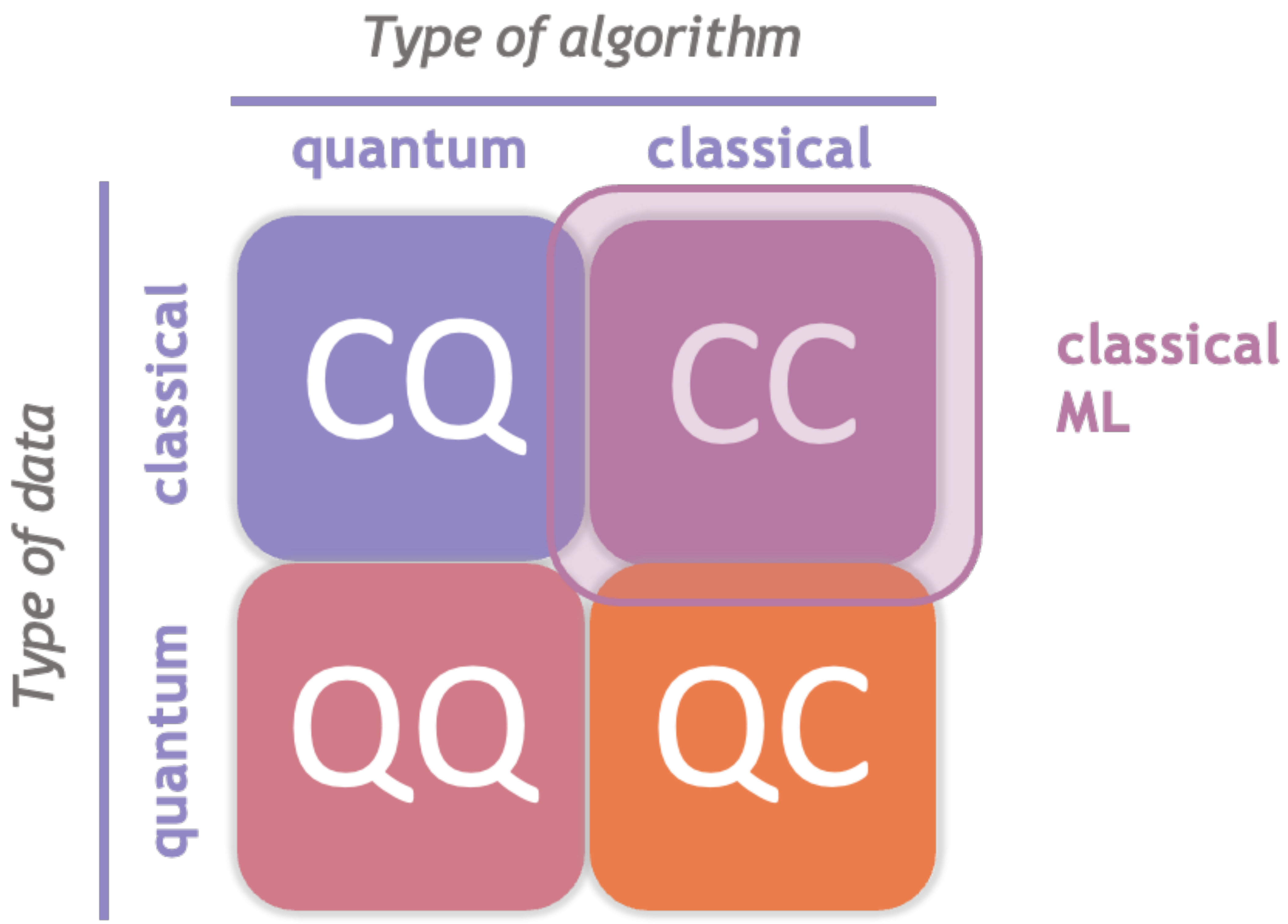


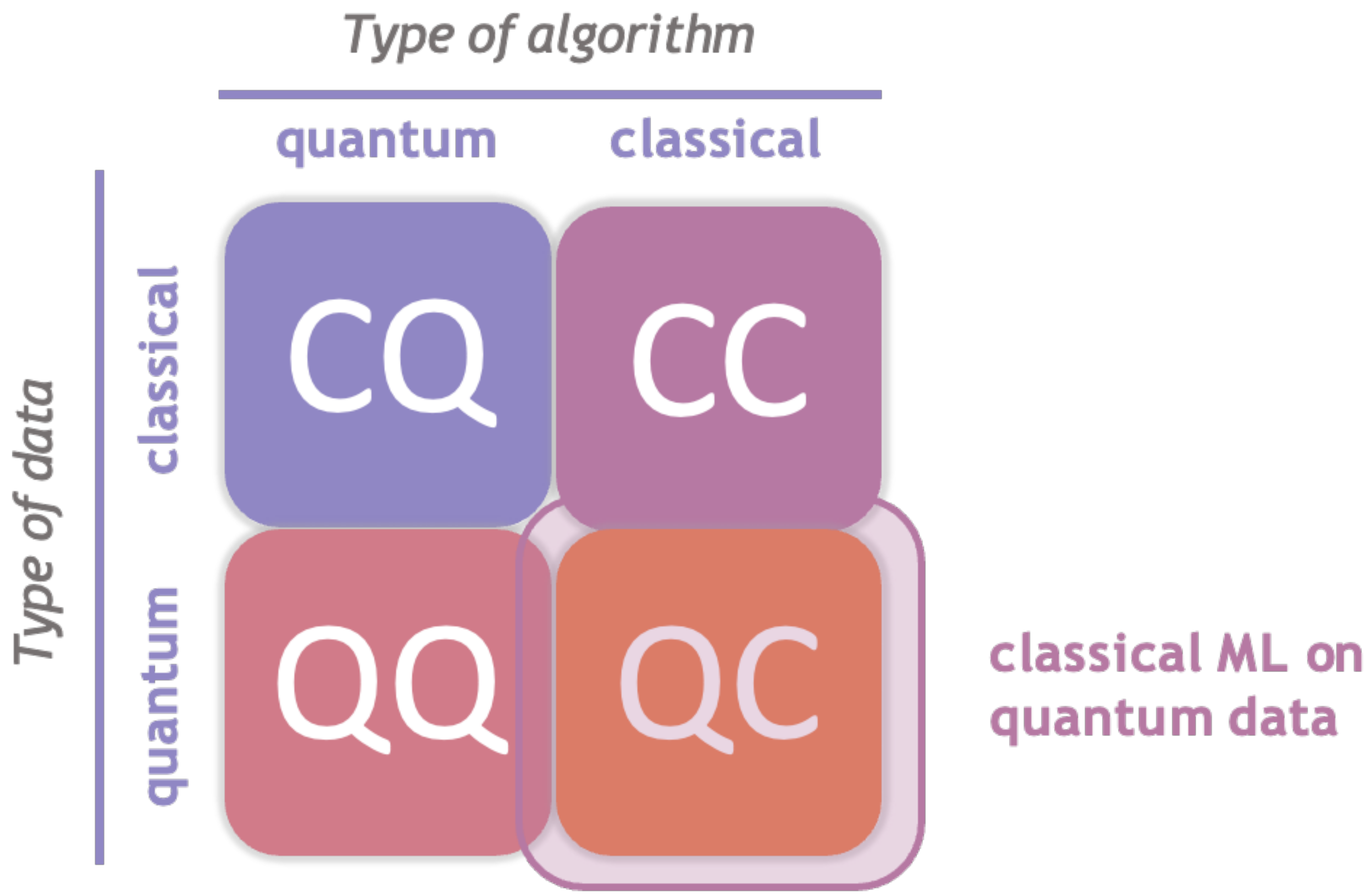
QCs can naturally solve certain problems with complex relations between inputs that can be incredibly hard for traditional, or "classical", computers. This suggest that learning models made on QC may be dramatically powerful for select applications, potentially boasting faster computation, better generalization on less data, or both.

Quantum Machine Learning

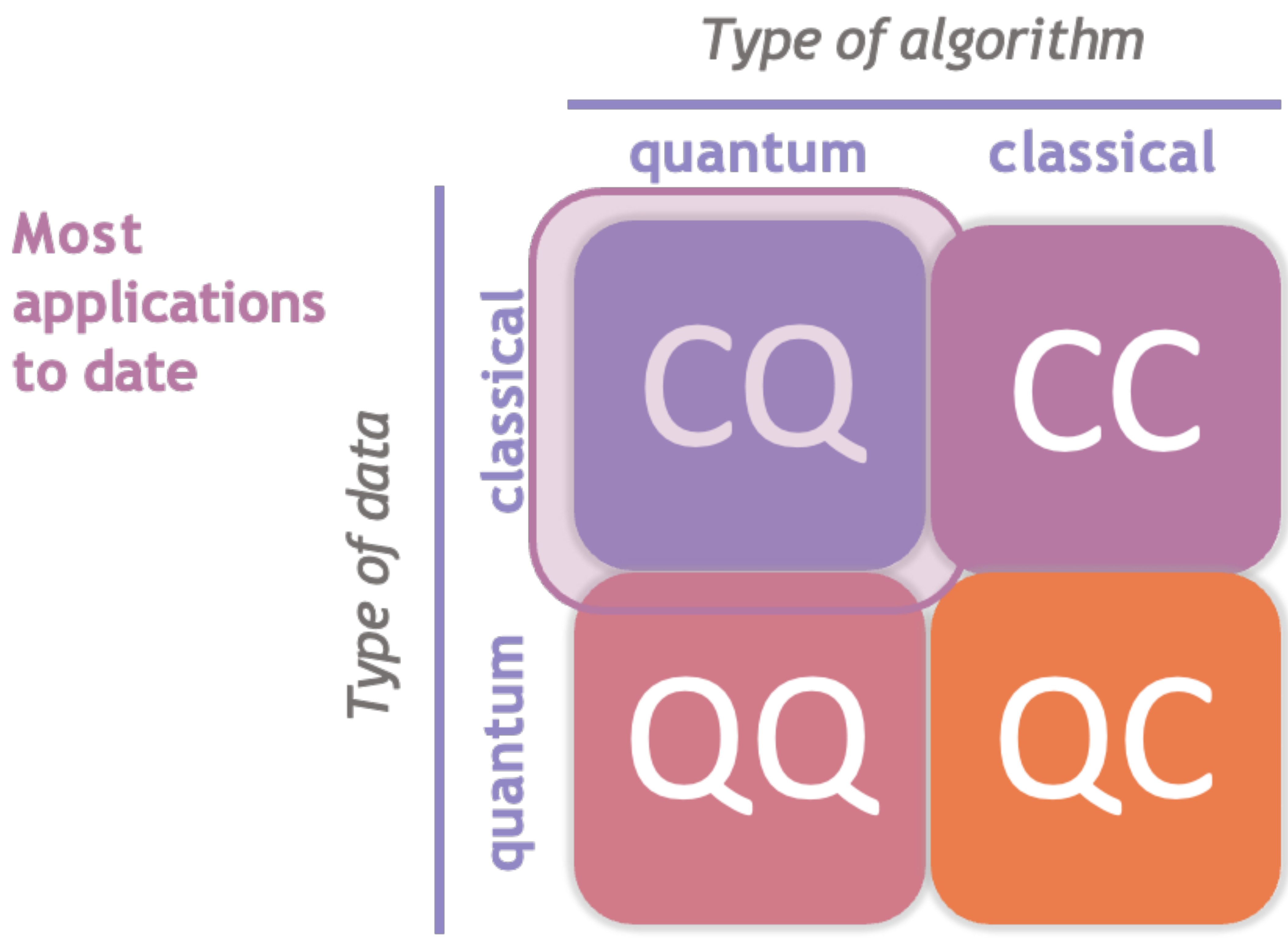


The intersection of quantum computing and ML is rich!

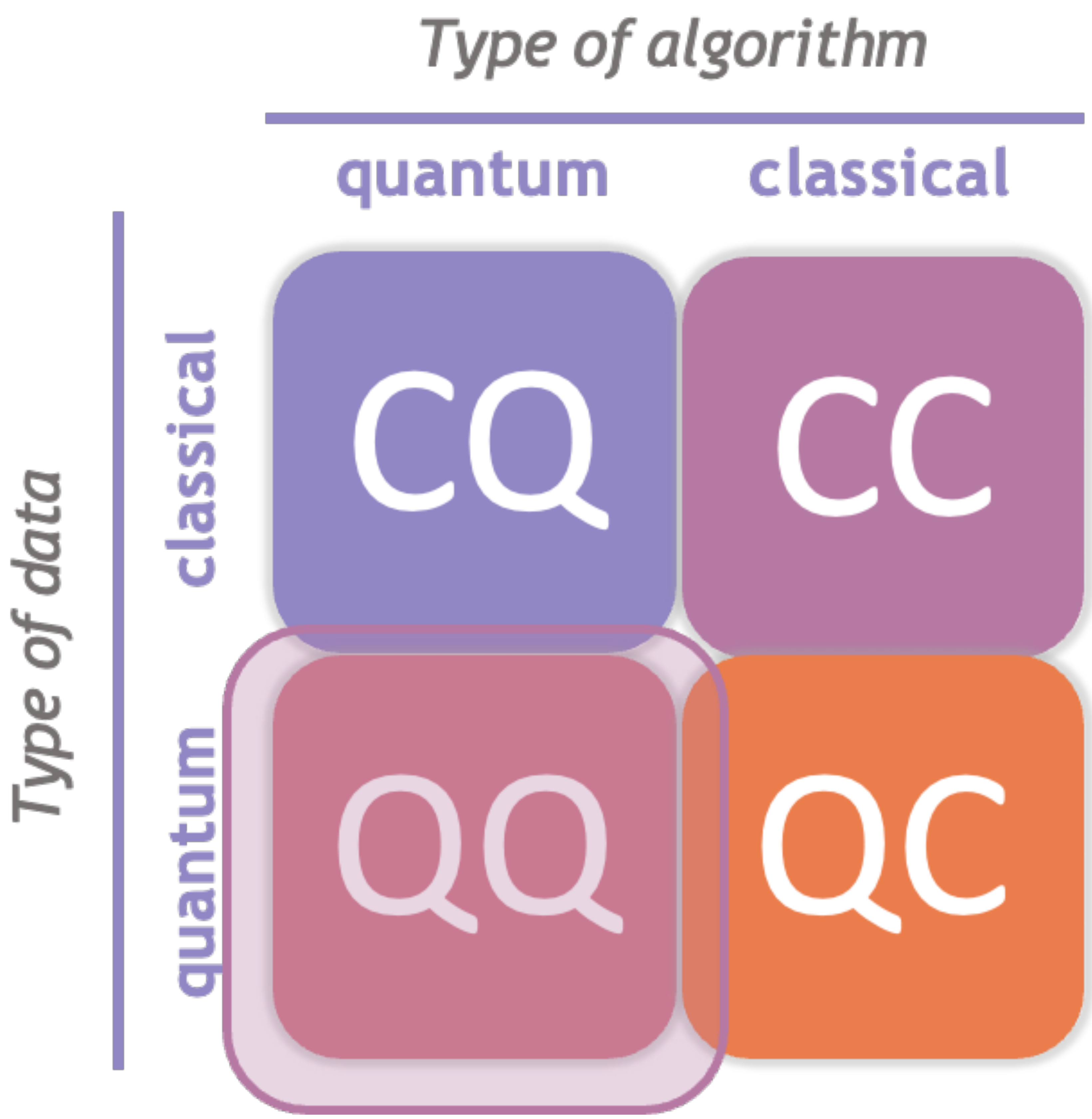
Quantum Machine Learning



Quantum Machine Learning



Quantum Machine Learning



Chemical simulation, Quantum matter simulation, Quantum control, Quantum networks, Quantum metrology

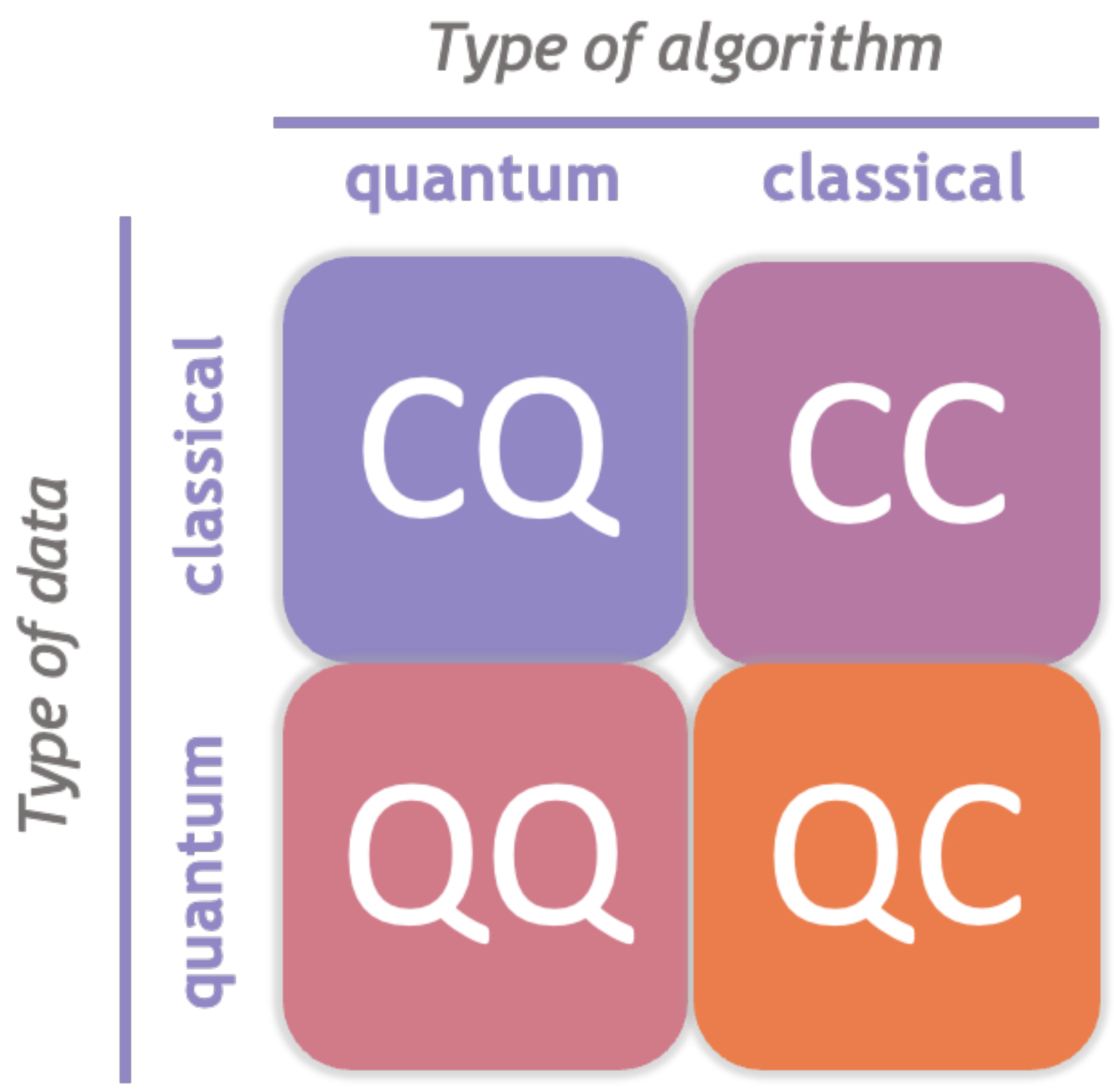
Quantum Machine Learning

The power of data

Very unlikely that QML will beat ML performance on classical data.

Data generated by a quantum circuit that is hard to simulate classically is not necessarily hard to learn for a classical model.

Datasets that are hard for classical models and easy for quantum models to learn do exist.



Understanding when a QC can help in a ML task depends not only on the task, but also on the data available, and a complete understanding of this must include both [*].

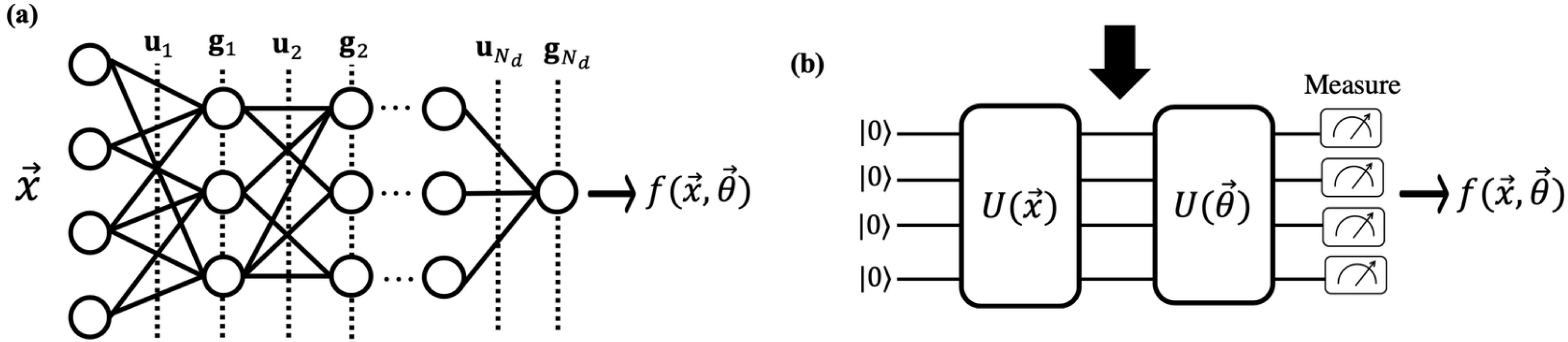
[*] Huang, HY., Broughton, M., Mohseni, M. et al. "Power of data in quantum machine learning," Nat Commun 12, 2631 (2021). https://doi.org/10.1038/s41467-021-22539-9

Quantum Machine Learning

In the NISQ Era

- Motivated by access to **cloud-based** processors and commercial applications.
- Developed for deployment on **NISQ** devices: Few qubits, Noisy, Low gate fidelity.
- 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



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

Benedetti, arXiv:1906.07682

Parameterized Quantum Circuits as ML Models

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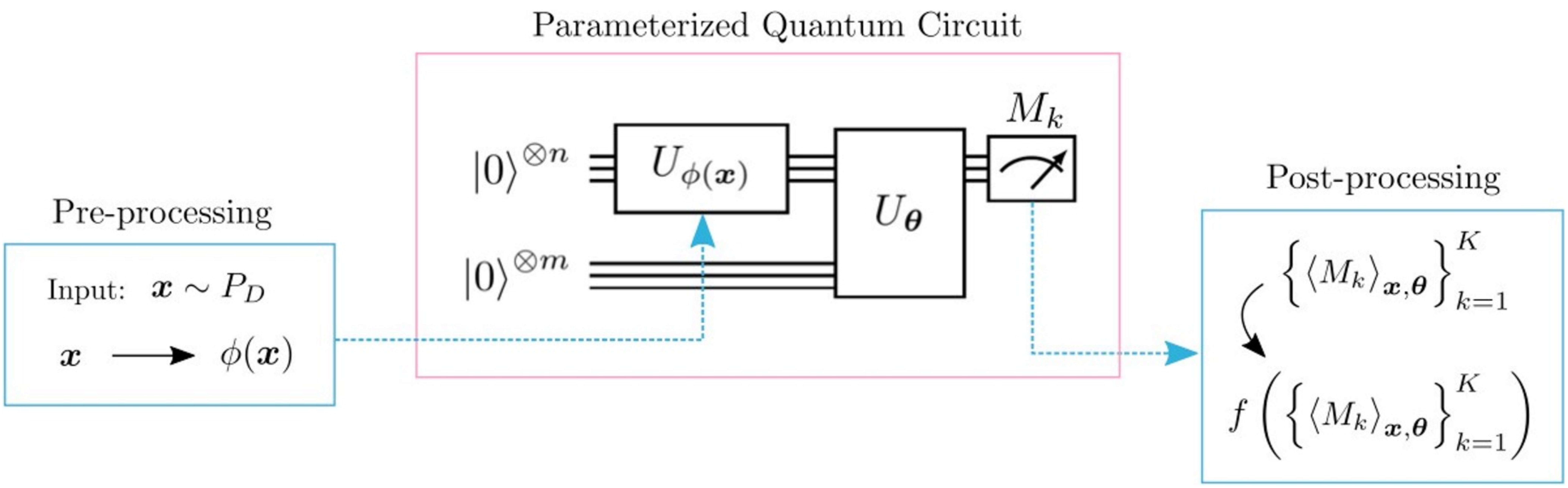

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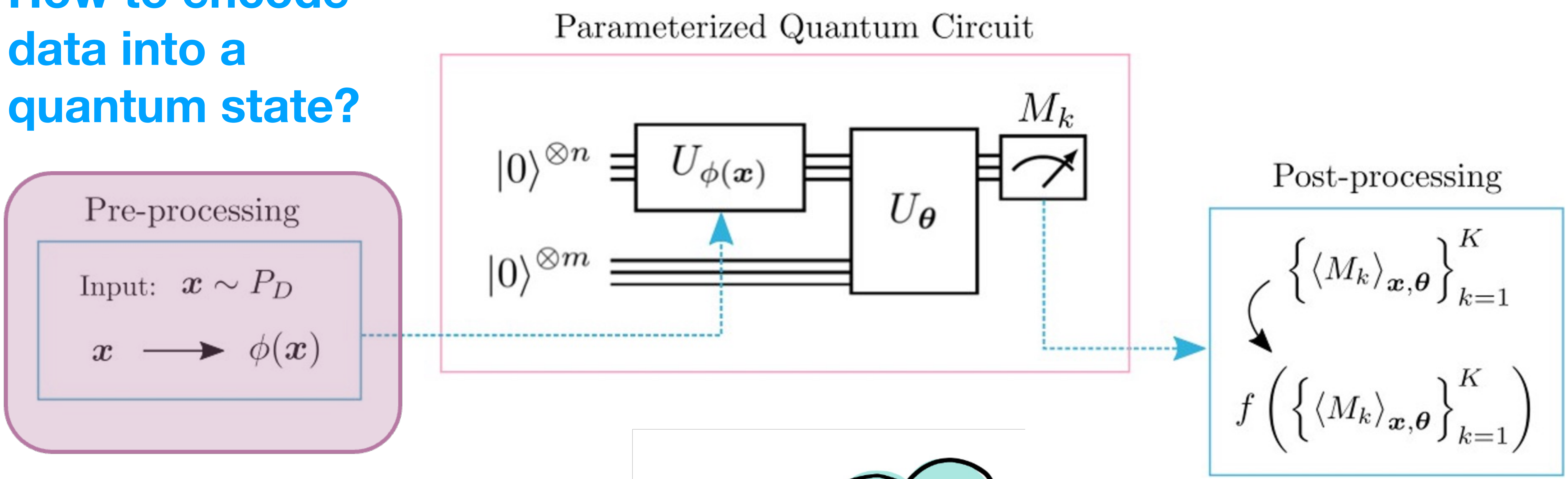
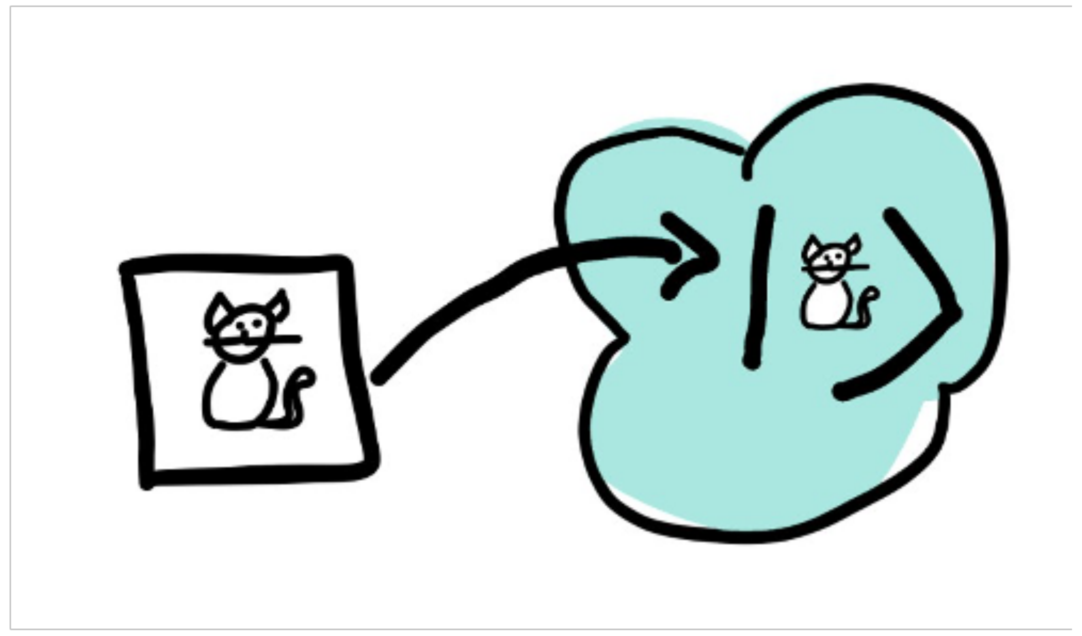
How to encode data into a quantum state?



1. Start from a feature vector x.
2. Optional: 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

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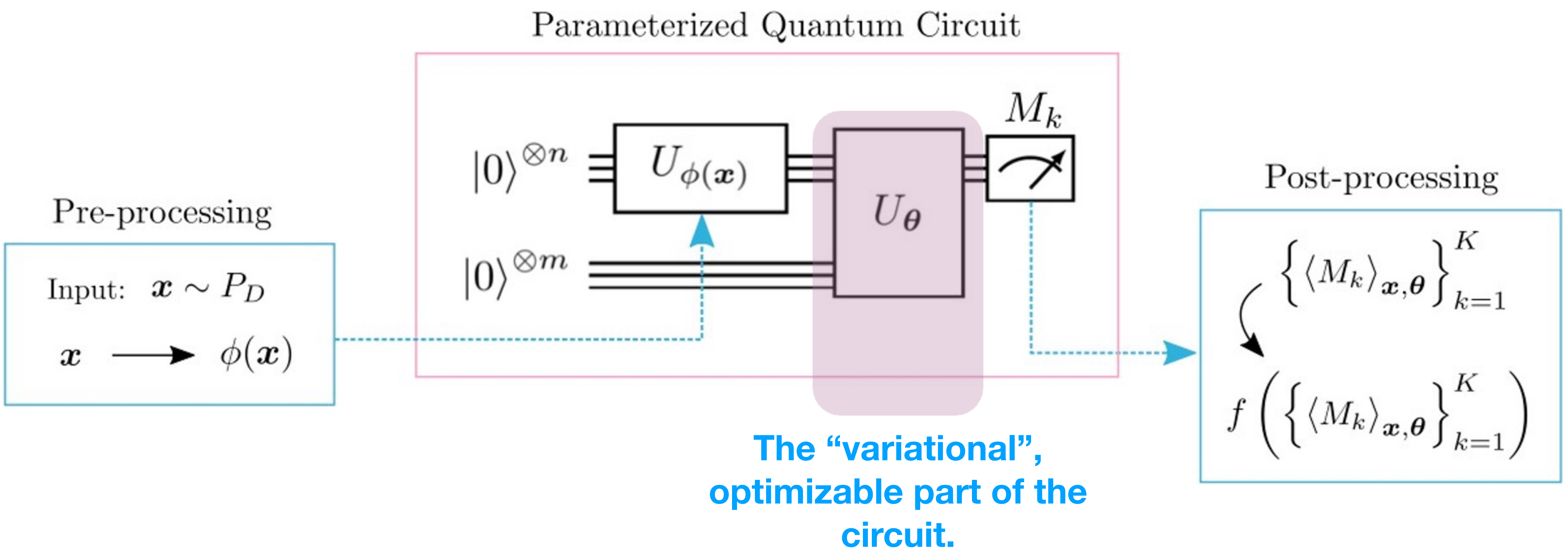

The "guess" or trial function is the unitary U parameterized by a set of free parameters θ that will be updated during training.

Parameterized Quantum Circuits as ML Models

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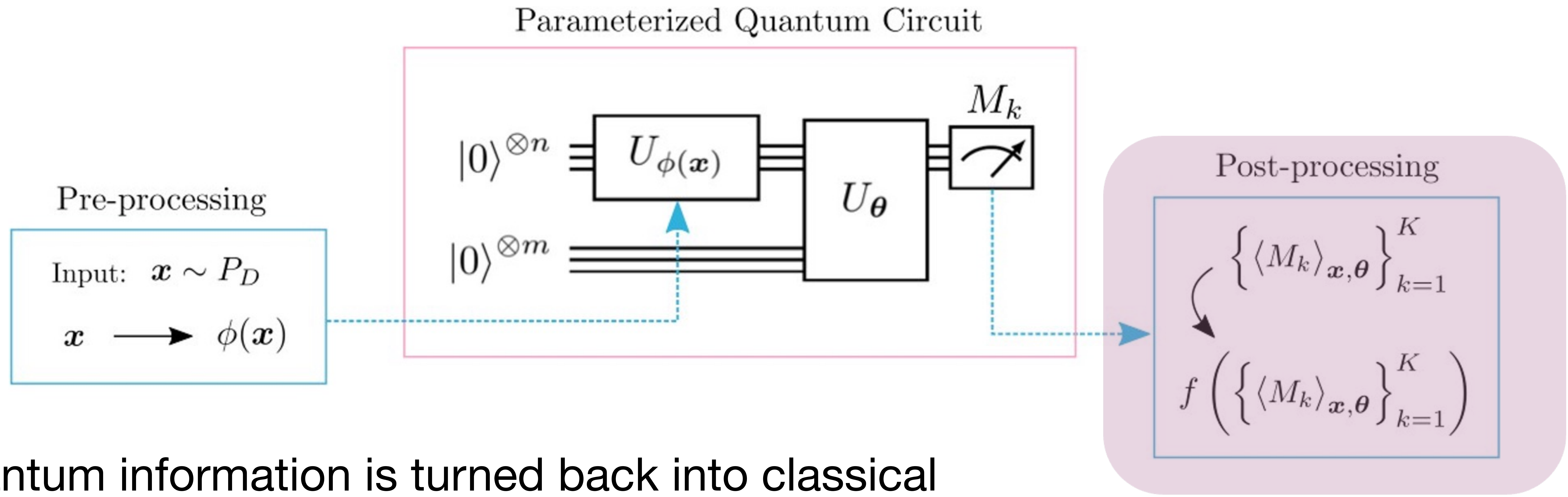


Quantum information is turned back into classical information by evaluating the expectation value of an observable, or measurement.

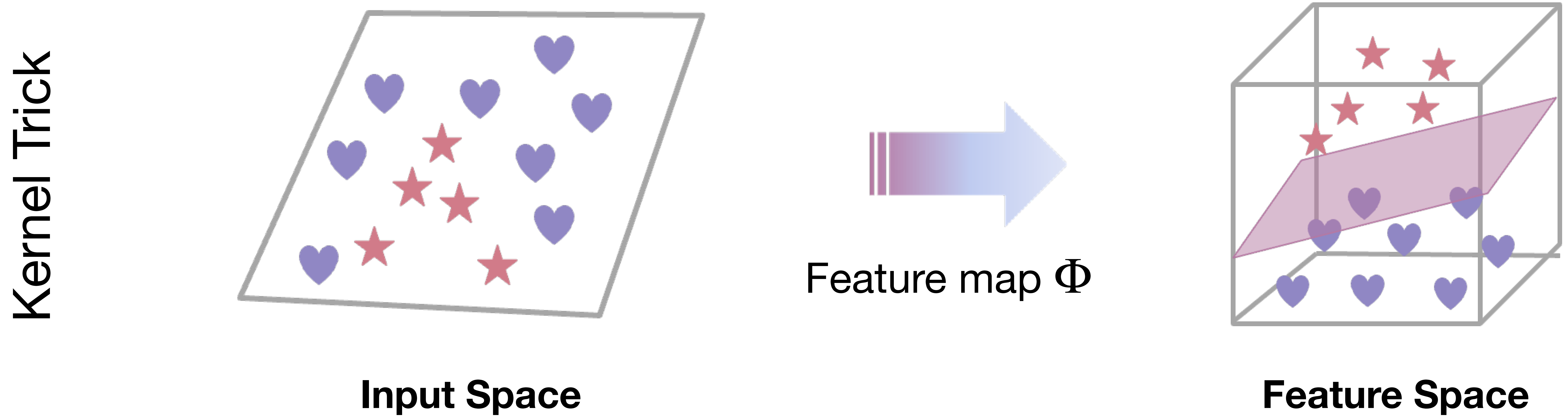
The measurement output is then used to construct a decision function, a probability distribution, a boundary, etc.

Applications

Supervised Learning with Kernel-based Quantum

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)*

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



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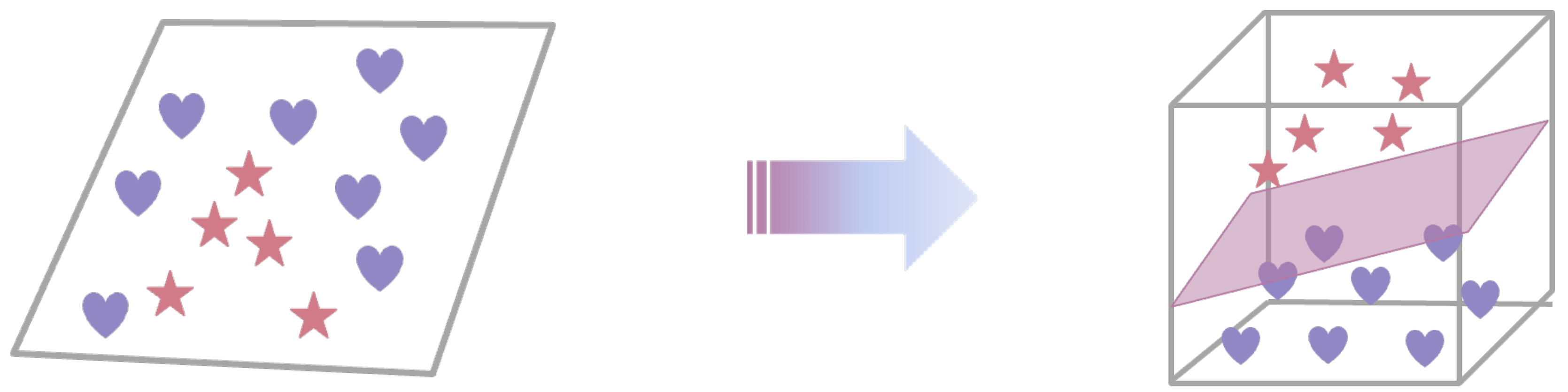
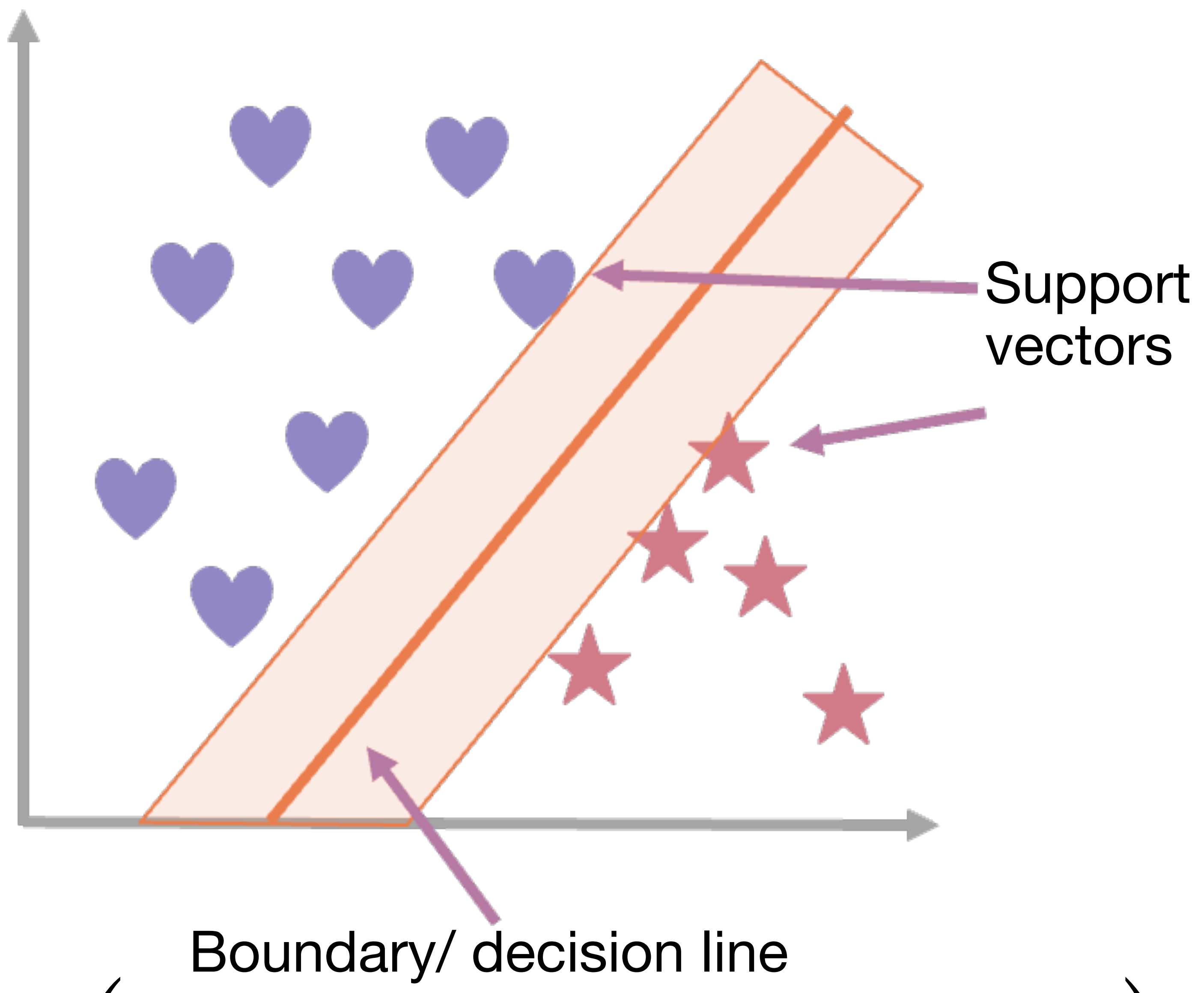


Support Vector Machine



To optimize a loss function of the form

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

Kernel

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

Supervised Learning with Kernel-based Quantum Models

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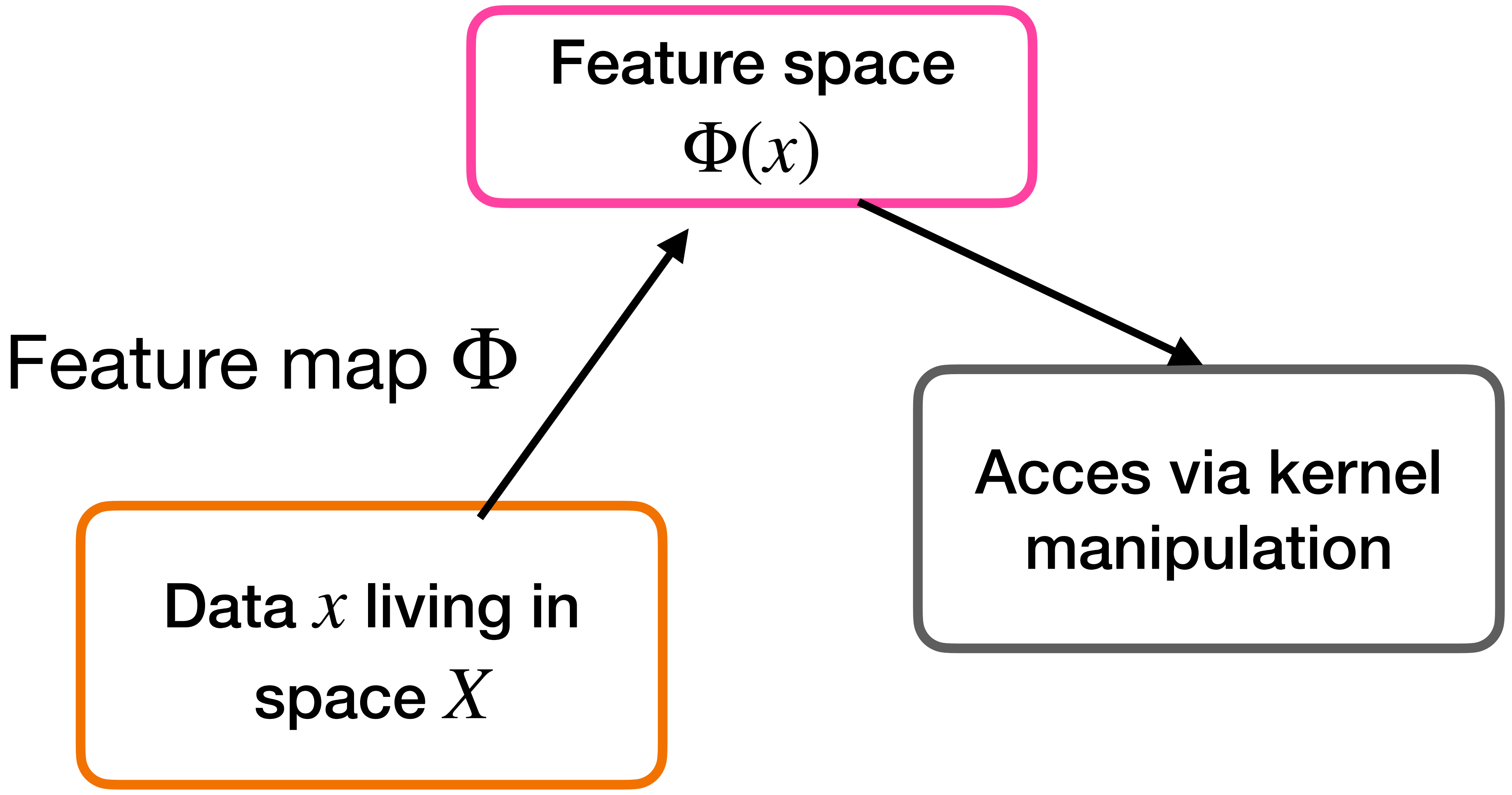
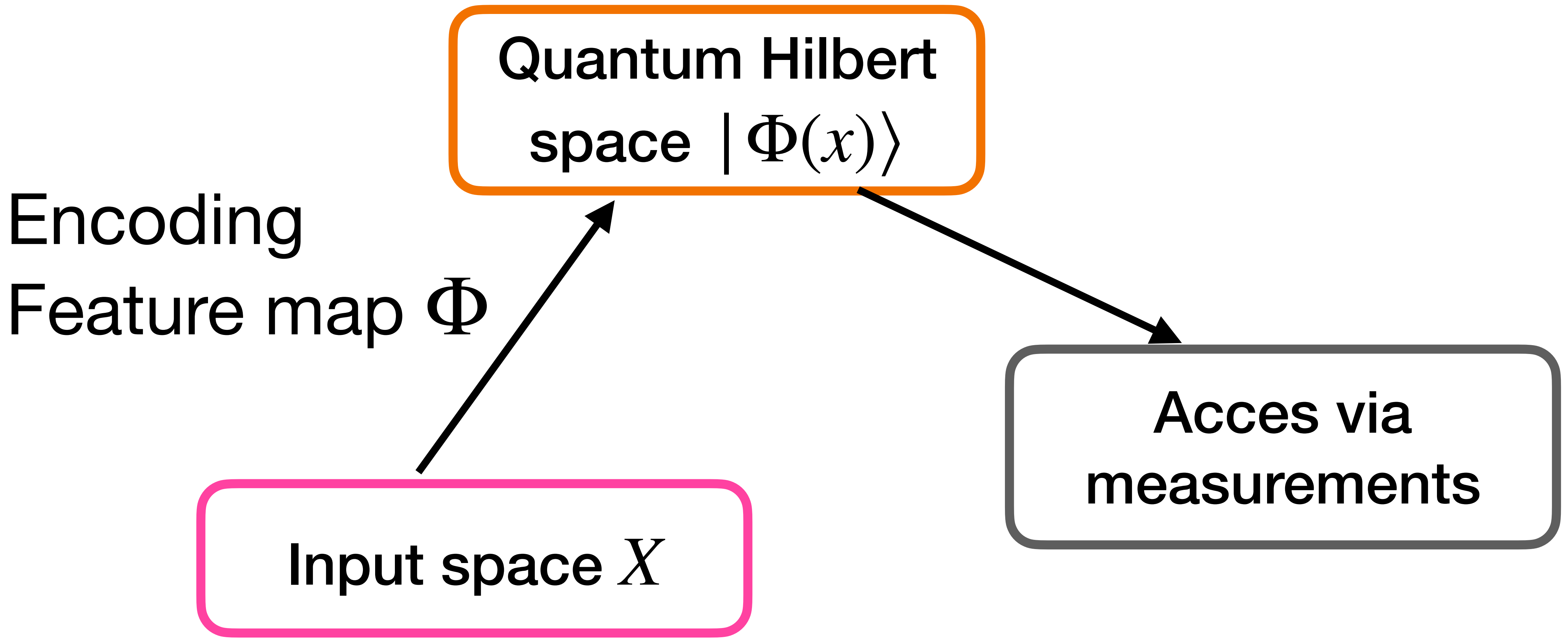
Kernel Methods



Quantum Machine Learning



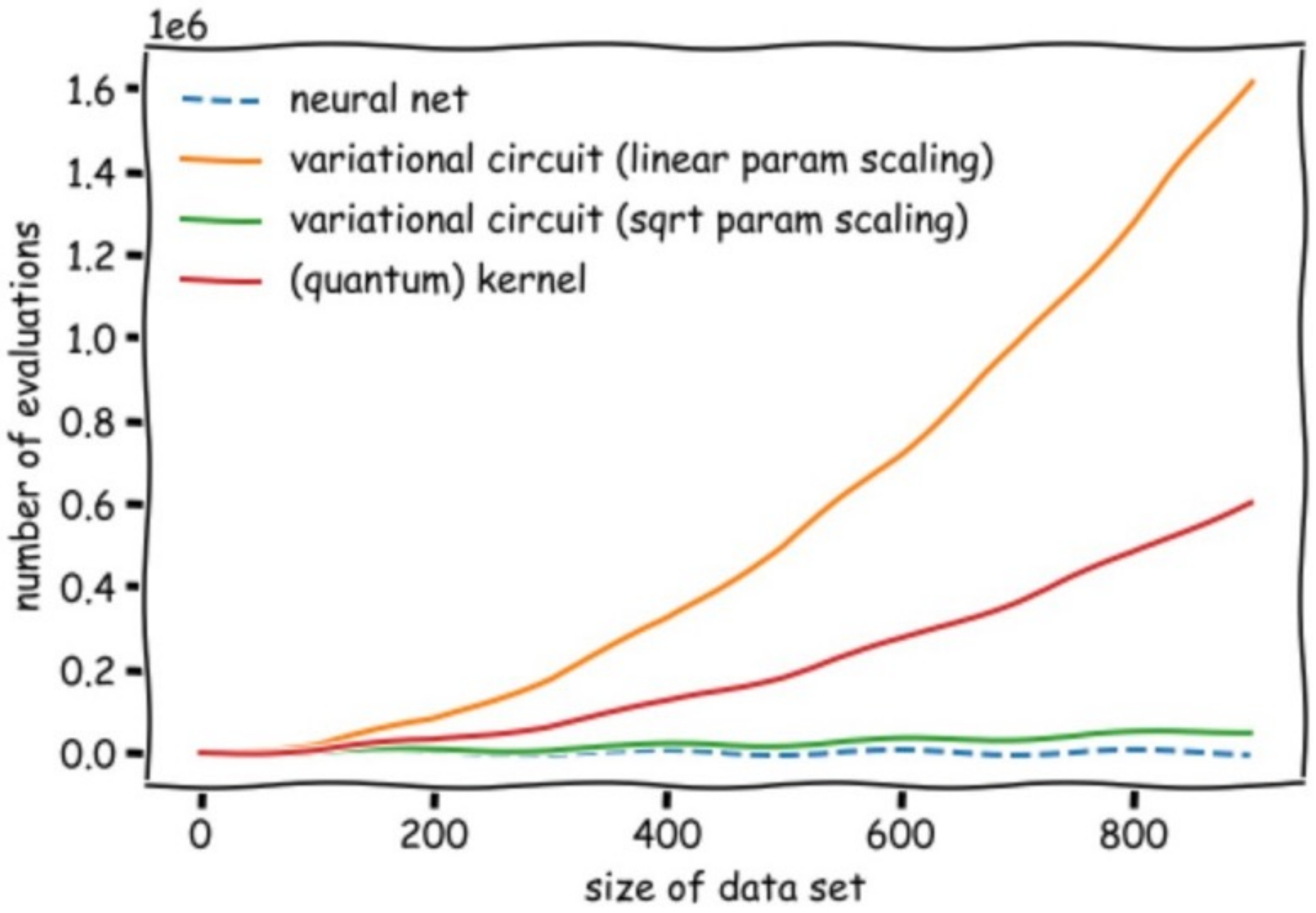
On Kernel-based Quantum Models

- **Kernel methods** are essentially based on feature maps that allow for *classification on a higher-dimensional space*.

- Quantum machine learning models based on kernel methods might provide an **advantage** when *the kernel is hard to estimate classically*.

- But… the efficiency of kernel-based methods compared to variational circuits depends on the number of parameters used in a variational model.

- Meaning that for specific applications, if the number of parameters scales linearly, most likely your application is better suited for a VQC.



Checkout PennyLane tutorial on “Kernel-based training of a quantum models with scikit- learn” https://pennylane.ai/qml/demos/tutorial_kernel_based_training.html

- **Unsupervised Generative Modeling**

- **Barren Plateaus, and how to avoid them**

Is Quantum Advantage the Right Goal for QML?

Based on the Perspective Manuscript by M. Schuld and N. Killoran, PRX Quantum 3, 030101 (2022)

- ML is a hard problem!

There is no rigorous basis for generalization.

NNs are sequences of linearand non-linear transformations, making them unwieldy for mathematical modeling.

- Once we add “quantumness”to the mix

We only have minimal access toempirical results from *“just running the algorithm”.*

We cannot say much about the behavior that quantum models will have at a scale beyond *what can be “simulated*”.

What architecture is best suited for a problem?

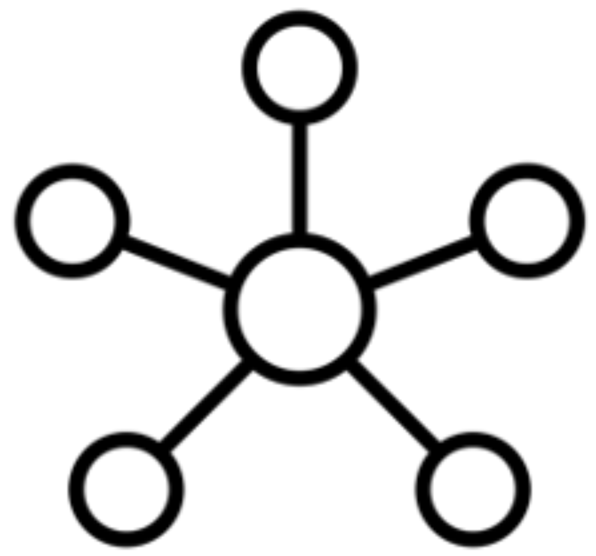
- **What affects trainability?**
- **Model expressibility**
- **Generalization power?**

”The question on whether quantum computers can really play a role in identifying practical ML application is still wide open, and It is unlikely to be decided by theoretical proofs or small-scale experiments”

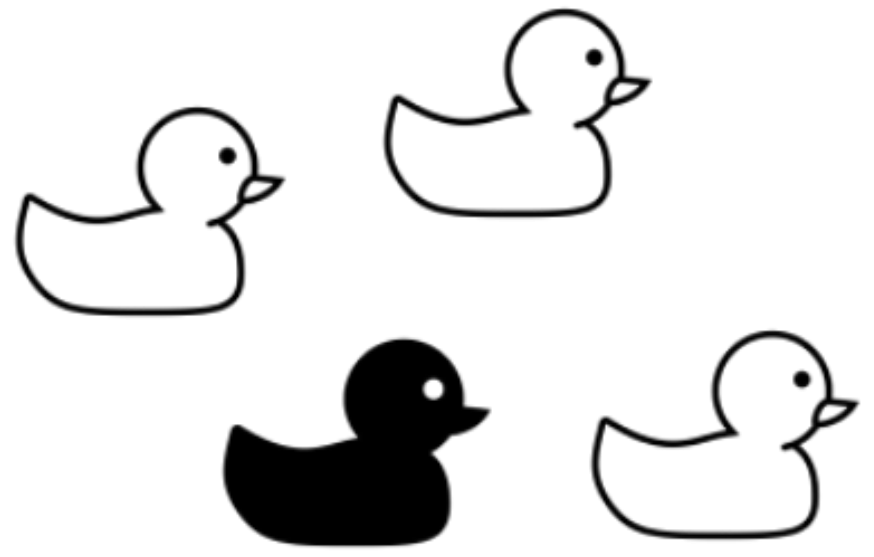
But also … what about?

Quantum Machine Learning on Quantum Data?

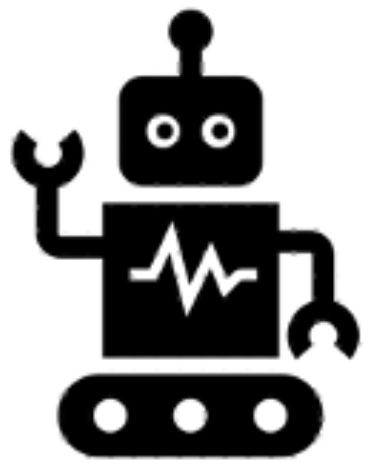
Ensemble learning methods for network of quantum sensors?



Anomaly detection?



System Control



Summary

1. Machine Learning algorithms based on parameterized quantum circuits are a prime candidate for near-term applications on noisy quantum computers. But…

2. We still don’t understand how these QML models compare, both mutually and to classical ML models.

3. There are several things I didn’t cover today, but I encourage you to read about them:

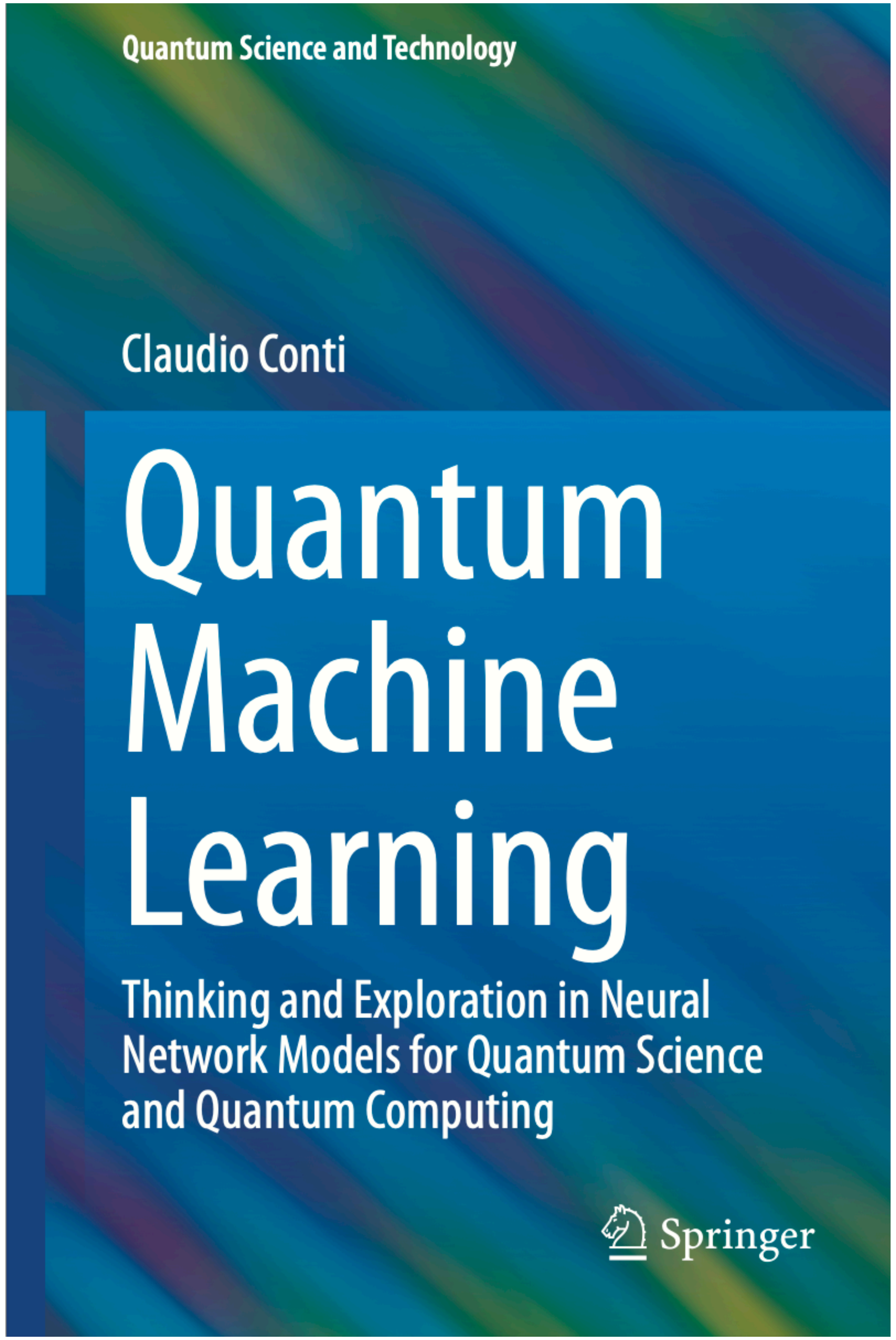
4. Continuous variable quantum machine learning

5. Tensor networks as ML models.

6. Its an exciting time for QML!

Thank you!

crbellor@unal.edu.co



Charla
Data-Driven Quantum Mechanics
Kernelizing Quantum Mechanics
Qubit Maps
Variational Quantum Algorithms and the Ising Model
Two-Qubit Ising Model and Entanglement
Phase Space Representation
States as Neural Networks
Gaussian Boson Sampling
Variational Circuits for Quantum Solitons