

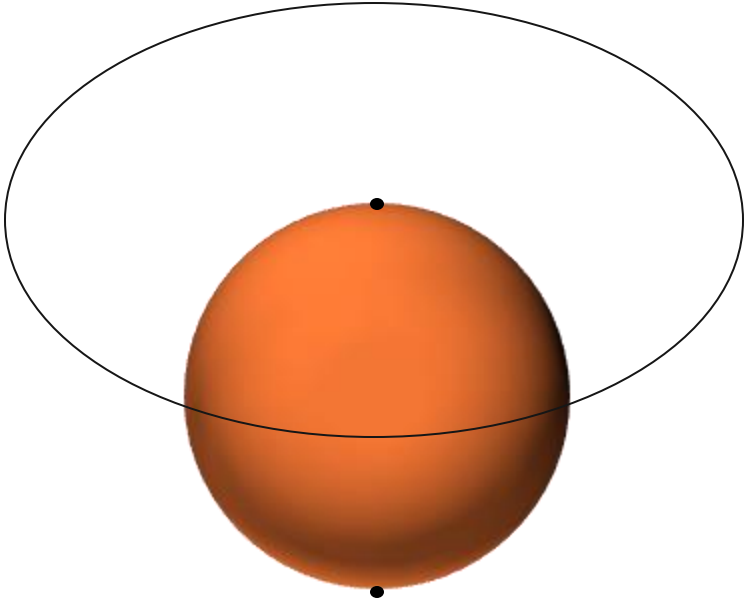
Current State of Quantum Machine Learning (QML)

Agenda

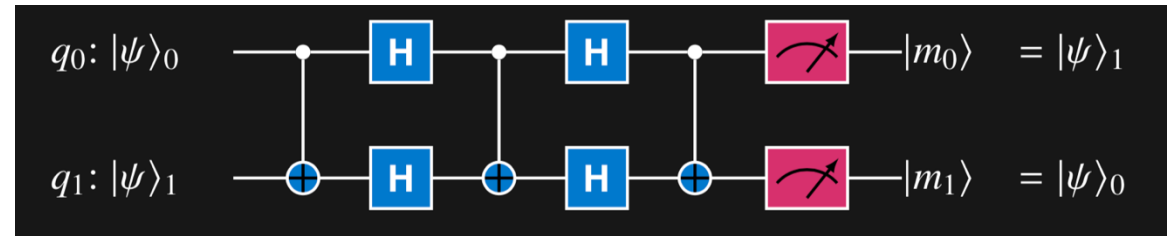
- Quantum Computing Overview
- Quantum Machine Learning
- Data Encoding and Mapping
- Near-term methods: QSVM, QNN, QGAN, PQK

Quantum Computing Overview

Quantum bits (qubits) and quantum circuits

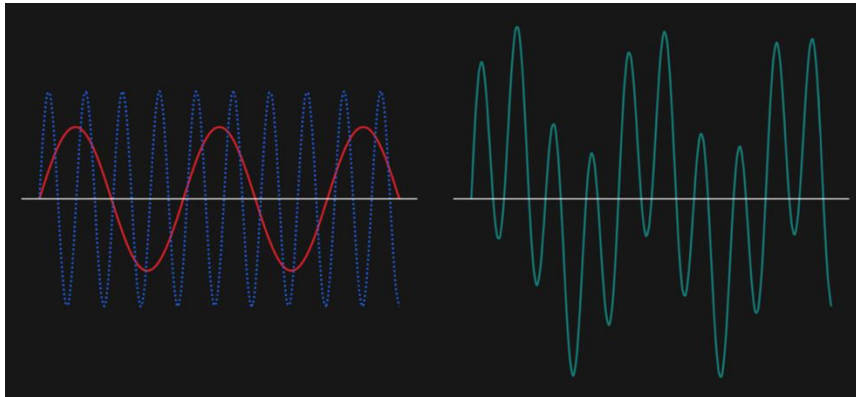


quantum bit qubit

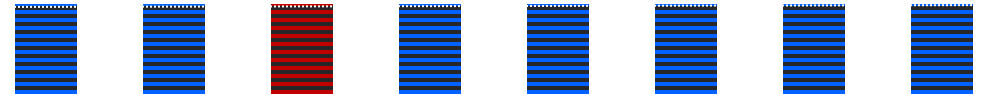


quantum circuit

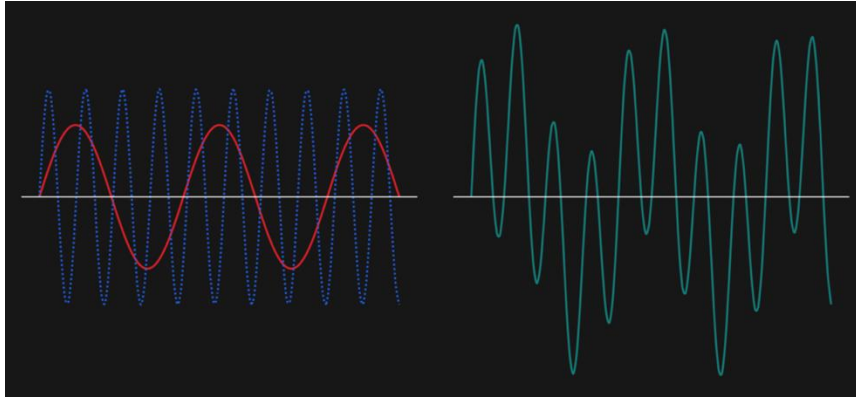
Quantum computing uses essential ideas from quantum mechanics



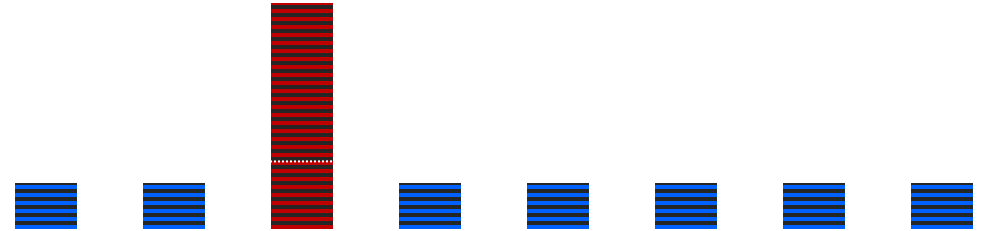
- Interference allows us to increase the probability of getting the right answer and decrease the chance of getting the wrong one.



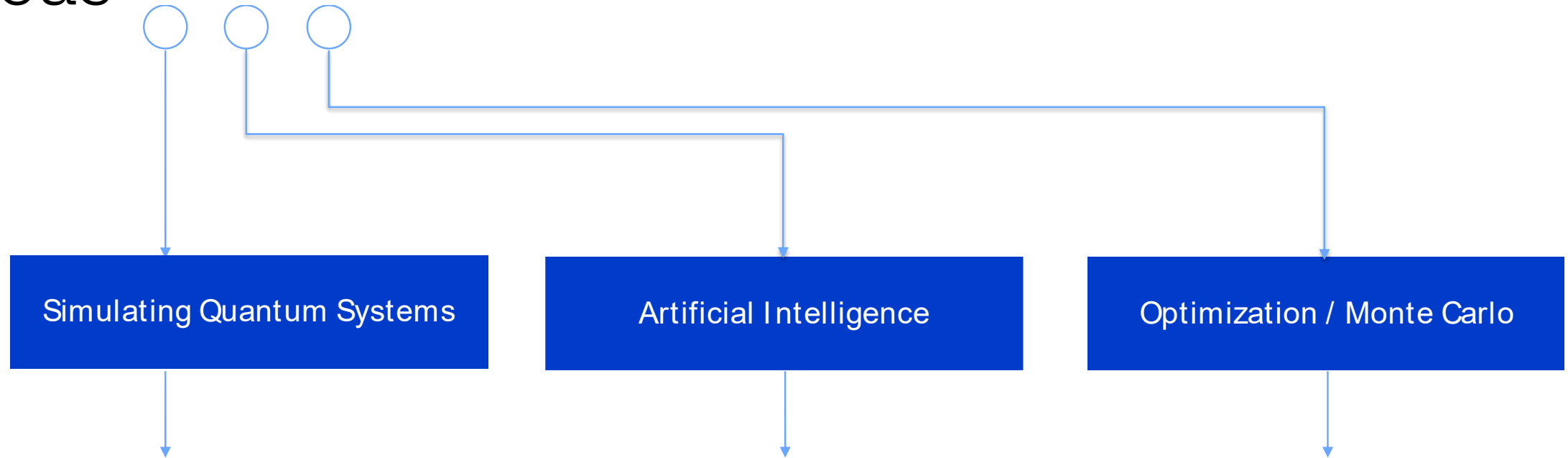
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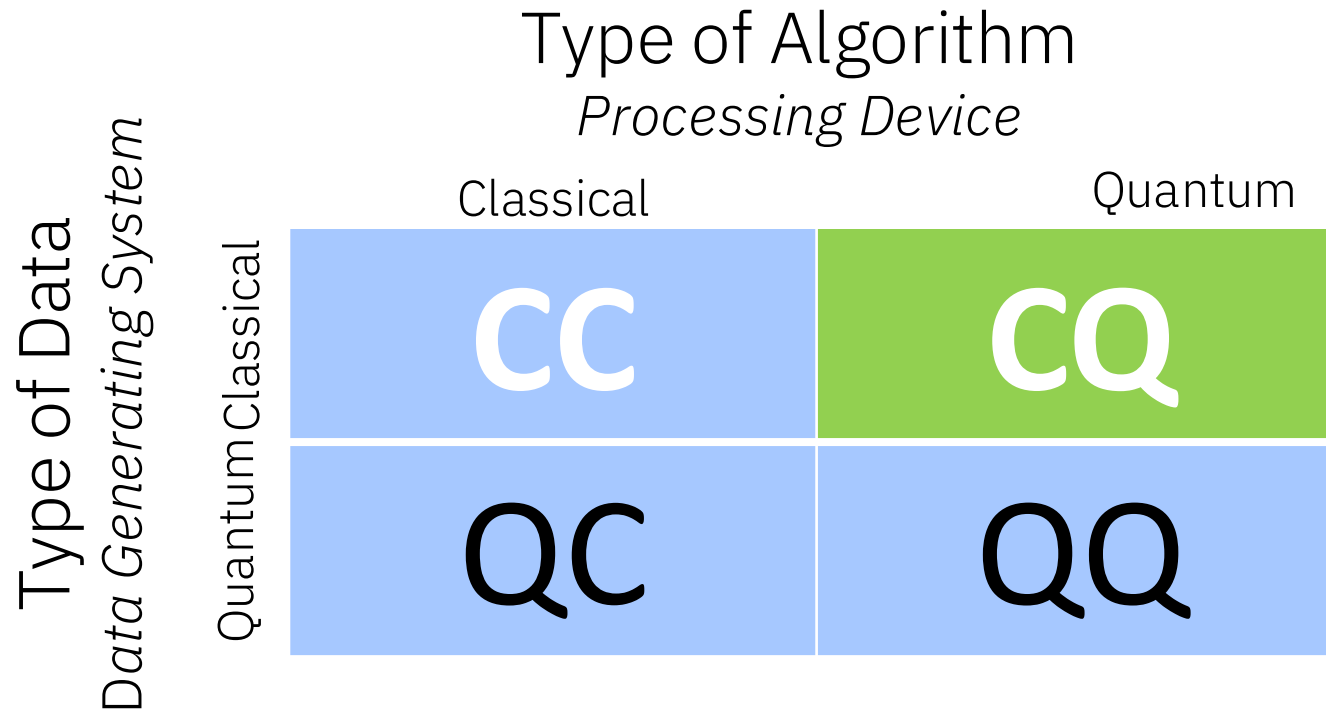


Quantum applications span three general areas



Quantum Machine Learning

Machine Learning and Quantum Machine Learning

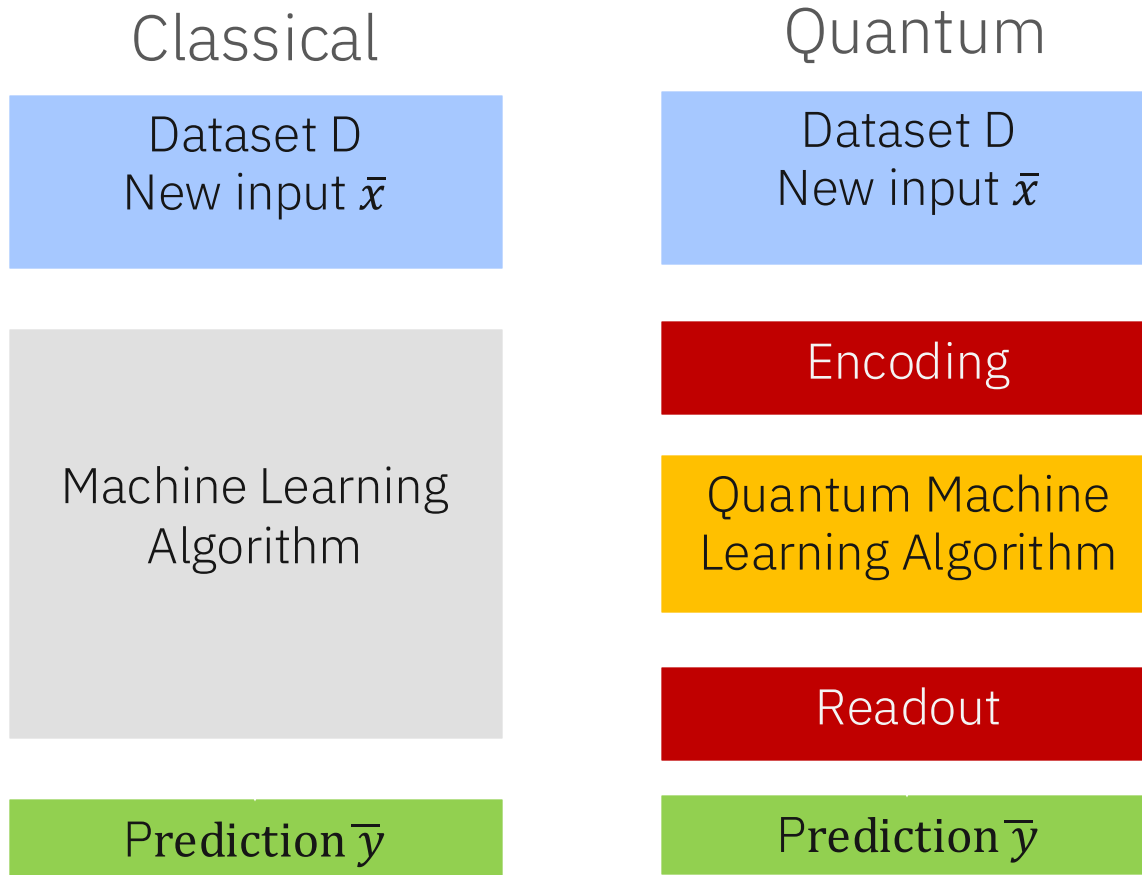


Maria Schuld, Francesco Petruccione
“Supervised Learning with Quantum Computers”, Page 6

Considerations beyond “the straightforward”

- *CC: in this context: Machine Learning based on methods borrowed from Quantum Information research, or “Quantum-Inspired”*
- *QC: how can Machine Learning help with Quantum Computing?*
- *CQ: synonym for QML. Data come from classical systems like text, images, time series, macro-economic variables*
- *Requires Quantum-Classical interface*
- *QQ: closely related to CQ. Data can be measured from quantum system or dataset can be Quantum States*

Quantum Machine Learning in a Nutshell



Data Encoding

One of the most important parts of QML Algorithms

*Frameworks, software and hardware that address the **interface** between classical memory and Quantum Device are key for runtime evaluations*

Encoding strategies

- *Qubit-Efficient* State Preparation
- Encode data in *Superposition*
- *Amplitude-Efficient* State Preparation

Example encoding methods

- Basis encoding
- Amplitude/angle encoding
- Encode dataset via *Hamiltonian*
- Data Encoding as a *Feature Map*

M. Schuld, F. Petruccione: Supervised Learning with Quantum Computers

M. Schuld, N. Killoran: arxiv 1803.07128

Near-Term and Fault-Tolerant Methods



Emerging Approach - [Third Wave](#)

- Based on deeper understanding of ML Potential of Quantum phenomena
- Combine the CML knowledge with Quantum Information Theory
- Train Quantum Models we cannot simulate any more ...
- **QUANTUM INSPIRED METHODS**

> 2021

Near Term Approach - [Second Wave](#)

- “What type of ML Model fits the physical characteristics of a small-scale Quantum Device?”
- New Models and Algorithms derived
- “Empirical” and “Heuristic” mindset
- **ISSUE: IS A CLASSICAL ML MINDSET SUFFICIENT... ?**

> 2017

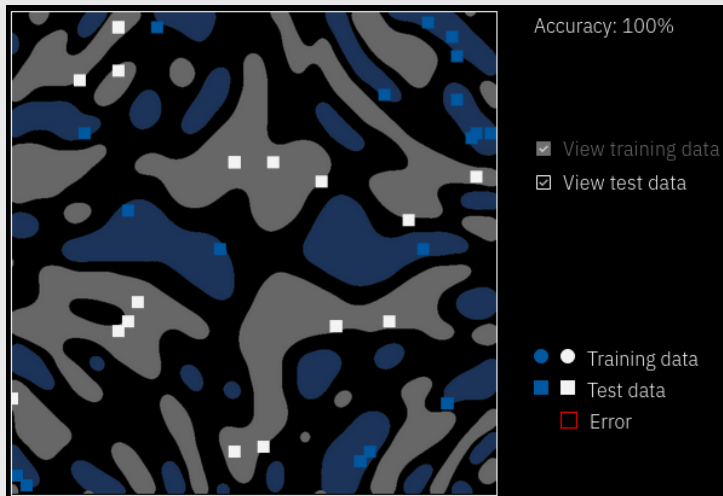
Long Term Benefit – [First Wave](#)

- Assumes Fault-Tolerant Quantum Computers
- Rather “Academic” and “Mathematical” mindset
- **ISSUE: WE ONLY HAVE NISQ TODAY ...**

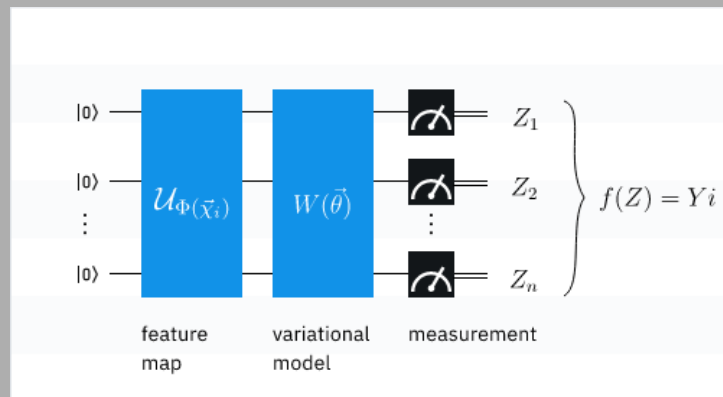
> 2013

Near-term QML algorithms

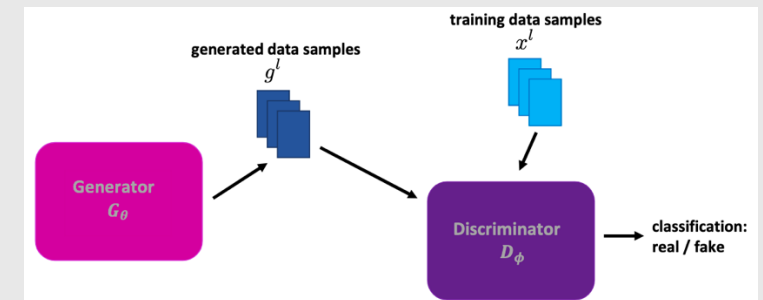
- Quantum SVM
 - Classification/regression tasks
 - Quantum kernel estimation method
 - Benefit: quantum feature space
- Key paper: Havlíček et al, *Nature* 567, pp 209–212 (2019)



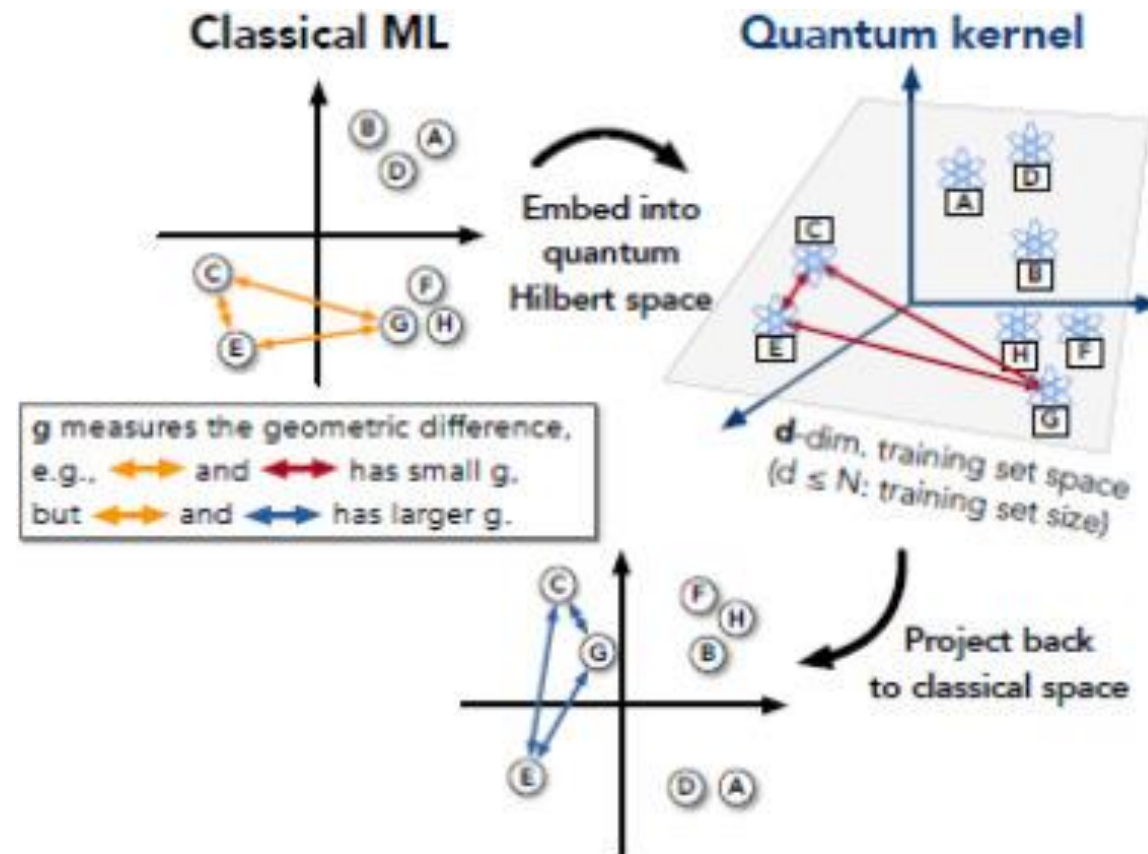
- Quantum Neural Networks
 - Classification/regression tasks
 - Variational quantum circuits
 - Benefits: model expressibility, resilience to barren plateaus
- Key paper: Abbas et al, *Nature Comp. Sci.* 1, pp 403–409 (2021)




- Quantum GANs
 - Data generation tasks
 - Quantum/classical neural networks
 - Benefits: efficient data sampling
- Key paper: Zoufal et al, *npj Quant. Info.* 5, no: 103 (2019)



Projected Quantum Kernel



Power of data in quantum machine learning

[Hsin-Yuan Huang](#), [Michael Broughton](#), [Masoud Mohseni](#), [Ryan Babbush](#), [Sergio Boixo](#), [Hartmut Neven](#) & [Jarrod R. McClean](#) 

[Nature Communications](#) **12**, Article number: 2631 (2021) | [Cite this article](#)

Classical

Dataset D
New input \bar{x}

Machine Learning
Algorithm

Prediction \bar{y}

Quantum

Dataset D
New input \bar{x}

Encoding

Quantum Machine
Learning Algorithm

Readout

Prediction \bar{y}



Quantum + Classical

Dataset D
New input \bar{x}

Encoding

Machine Learning
Algorithm

Prediction \bar{y}

Fault-Tolerant QML

2013

*Are Quantum Computers
“better” at Machine Learning
than Classical Computers?*

- “Traditional Approach” to QML, assuming abundance of perfect Qubits ☺
- NOT novel methods, but novel implementations of the SAME METHODS
- Quality of Algorithm judged thru asymptotic computational complexity

arXiv:1307.0411 (quant-ph)

[Submitted on 1 Jul 2013 (v1), last revised 4 Nov 2013 (this version, v2)]

**Quantum algorithms for supervised and
unsupervised machine learning**

Seth Lloyd, Masoud Mohseni, Patrick Rebentrost

- **Quantum ‘BLAS’**
- Amplitude Encoding
- Runtime: $O(\log(N.M))$ with $N = 2^n$

- **HHL: Invert Data Matrix:**
- $w = (X^T X)^{-1} X^T y$
- *Linear Regression*
- [Quantum Data Fitting - N. Wiebe, D. Braun, S. Lloyd - 2012]

- **SVMs: Invert Kernel Matrix**
- *Classification*
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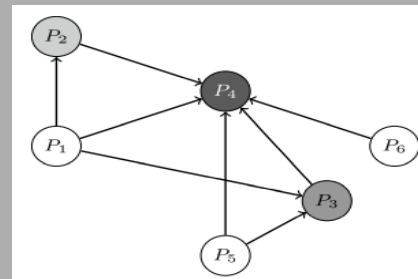
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- **Based on Grover’s Search**
- Amplitude Amplification
- Speedup: $O(n^2)$
- **Perceptron + Amplitude Amplification**
- [Quantum Perceptron Models – N. Wiebe, A. Kapor, K. Svore - 2016]
- **Quantum Walks (E.g.: PageRank)**
- [Quantum speed-up of Markov chain- based algorithms]



Fault-Tolerant QML

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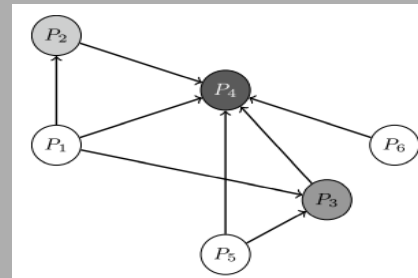
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• Probabilistic Methods

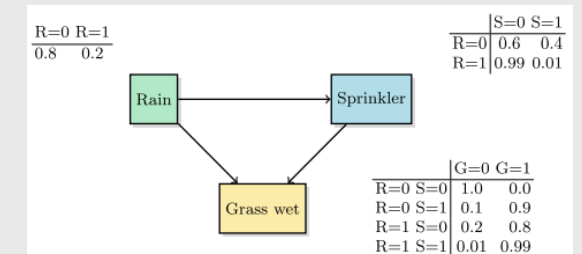
- Measurements sampled from classical probability distributions

• Bayesian Net

- Elegant State Preparation

- Runtime is $O(n^2)$ better than classical rejection sampling

• [Quantum inference on Bayesian Networks, G H Low, T J Yoder, I L Chuang - 2014]



Data Encoding and Mapping

Encoding Data

- **Basis Encoding**

Encode each n -bit feature into n qubits

$$x = (b_{n-1}, \dots, b_1, b_0) \rightarrow |x\rangle = |b_{n-1}, \dots, b_1, b_0\rangle$$

Combine M data points in superposition

- **Amplitude Encoding**

Encode into quantum state amplitudes

$$x = \begin{bmatrix} x_0 \\ \vdots \\ x_{N-1} \end{bmatrix} \rightarrow |\psi_x\rangle = \sum_{j=0}^{N-1} x_j |j\rangle$$

Combine M data points in superposition

- **Angle Encoding**

Encode values into qubit rotation angles

$$|x\rangle = \bigotimes_{i=0}^{N-1} (\cos(x_i) |0\rangle + \sin(x_i) |1\rangle)$$

- **Arbitrary Encoding (Feature Map)**

Encode N features on N rotation gates in constant-depth circuit with n qubits

$$x = \begin{bmatrix} x_0 \\ \vdots \\ x_{N-1} \end{bmatrix} \rightarrow |\psi_x\rangle = \mathcal{U}_{\Phi(x)} |0\rangle$$

Encoding	# Qubits	State prep runtime
Basis	nN	$O(N)$
Amplitude	$\log(N)$	$\frac{O(N)}{O(\log(N))}$
Angle	N	$O(N)$
Arbitrary	n	$O(N)$

N features each

Quantum feature map - Simplistic

- **Process**

- Apply H gates on all qubits
- Apply parameterized Pauli rotations gates for each feature x_i
- Repeat k times

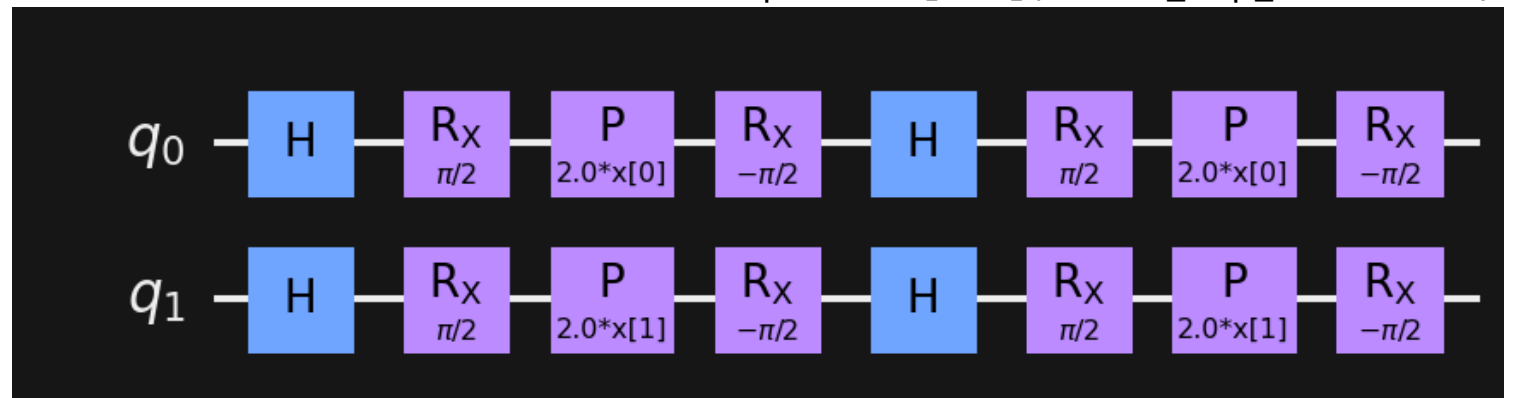
- **Pro:** Simple to implement
- **Con:** Does not exploit high dimensionality

Encoded state: $|\Phi(x)\rangle = \mathcal{U}_{\Phi(x)}|0\rangle$

$$\mathcal{U}_{\Phi(x)} = (U_{\Phi(x)} H^{\otimes n})^d$$

$$U_{\Phi(x)} = \exp\left(i \sum_i \underbrace{\phi_i(x) P_i}_{\text{Pauli rotation operator}} + \dots\right)$$

```
feature_map = PauliFeatureMap(feature_dimension=2, reps=2,
                               entanglement='linear', alpha=2.0,
                               paulis=['Y'], data_map_func=None)
```



Quantum feature map - Complex

- Process

- Apply H gates on all qubits
- Apply entangling gates and Pauli rotations gates for each feature x_i
- Repeat k times

$$|\Phi(x)\rangle = \mathcal{U}_{\Phi(x)}|0\rangle$$

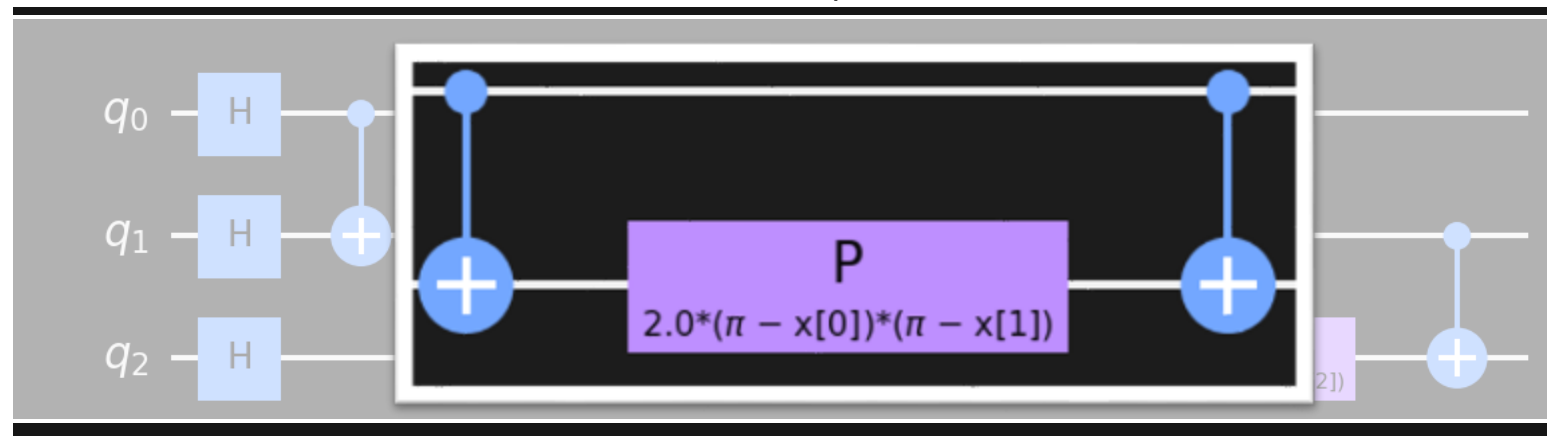
$$\mathcal{U}_{\Phi(x)} = (U_{\Phi(x)} H^{\otimes n})^d$$

$$U_{\Phi(x)} = \exp\left(i \sum_i \phi_i(x) P_i + i \sum_{i,j} \underbrace{\phi_{i,j}(x) P_{ij}}_{\text{2-qubit Pauli rotation operator}} + \dots\right)$$

2-qubit Pauli rotation operator

```
feature_map = PauliFeatureMap(feature_dimension=3, reps=1,  
                               entanglement='linear', alpha=2.0,  
                               paulis=['ZZ'])
```

- **Pro:** Exploits entanglement
- **Con:** Adds more gates



Quantum feature map – Complex (2)

- **Process**

- Apply H gates on all qubits
- Apply entangling gates and Pauli rotations gates for each feature x_i
- Repeat k times

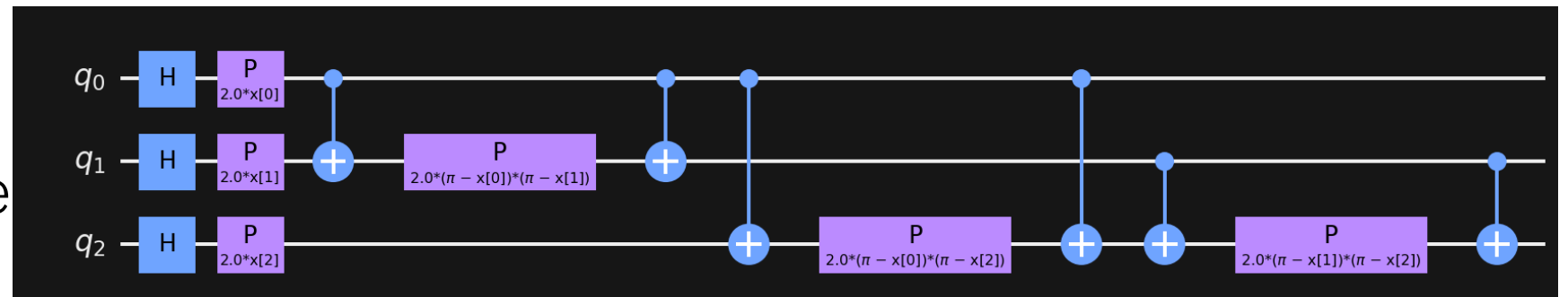
$$|\Phi(x)\rangle = \mathcal{U}_{\Phi(x)}|0\rangle$$

$$\mathcal{U}_{\Phi(x)} = (U_{\Phi(x)} H^{\otimes n})^d$$

$$U_{\Phi(x)} = \exp\left(i \sum_i \phi_i(x) P_i + i \sum_{i,j} \phi_{i,j}(x) P_{ij} + \dots\right)$$

```
feature_map = PauliFeatureMap(feature_dimension=3, reps=1,  
                               entanglement='full', alpha=2.0,  
                               paulis=['Z', 'ZZ'])
```

- **Pro:** Exploits entanglement
- **Con:** Adds more gate

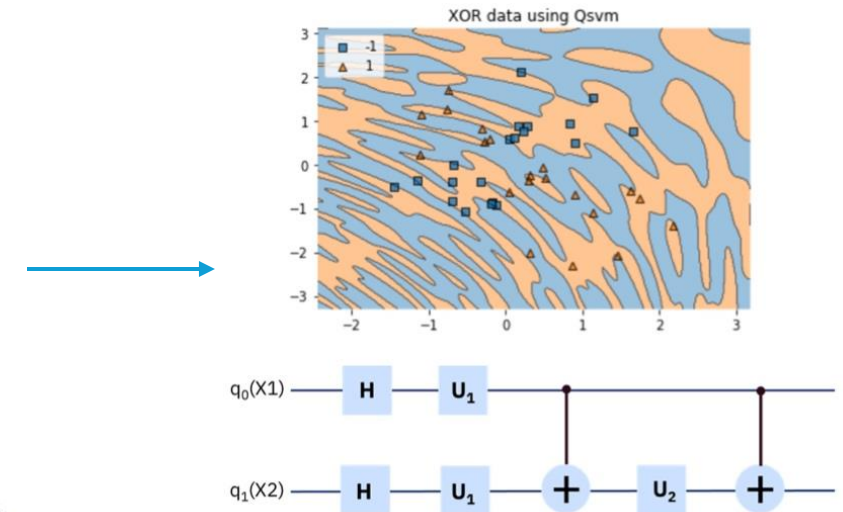
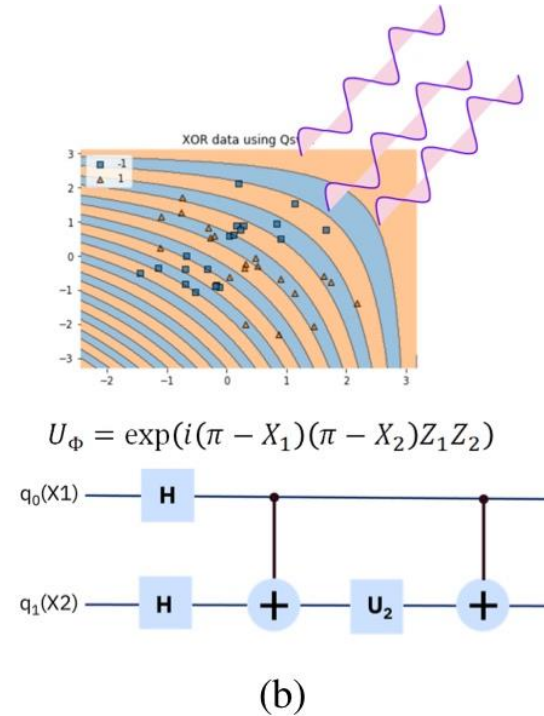
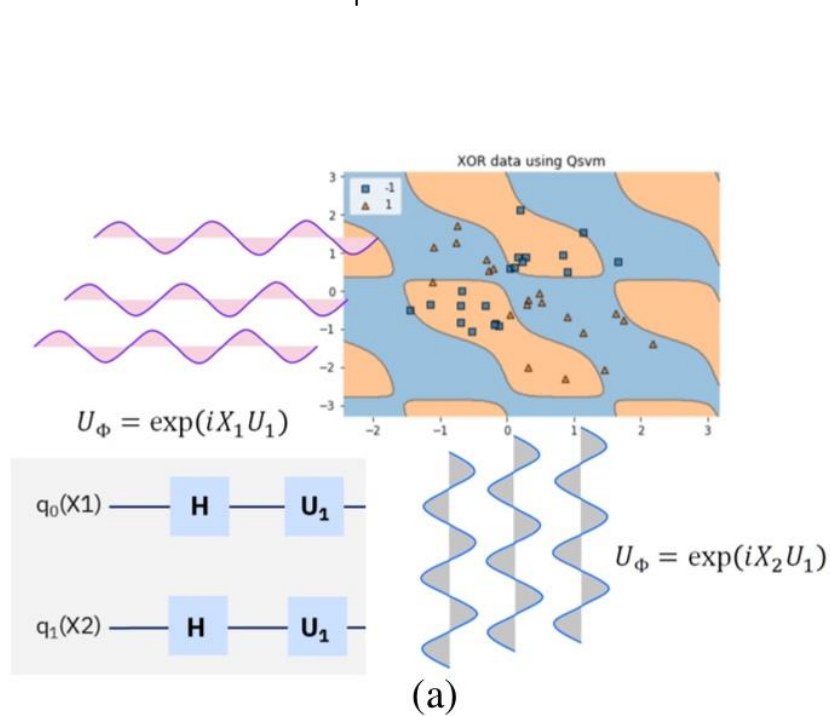


Quantum feature maps

Simple rotations

Entangled unitary rotations

Simple and Entangled unitary rotations



Park et al, arXiv: 2012.07725v1

Thank you