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Introduction to Quantum Machine Learning

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Karthiganesh Durai

Founder & CEO, KwantumG Research Labs Pvt Ltd, Bengaluru

Co-Founder, Quantum Computing India, Bengaluru

Professor of Practice, NMIT, Bengaluru

About Me

Karthiganesh Durai

Founder & CEO, KwantumG Research Labs Pvt Ltd, Bengaluru
Senior Quantum Software Consultant, BosonQ Psi Corp., New York 2022-2023
Professor of Practice, Nitte Meenakshi Institute of Technology, Bengaluru
Visiting faculty in SRM Univ, Chennai, VIT Chennai and Naval War College, Goa

- Master in Computer Applications, NIELIT
- Master in Business Administration, Puducherry University
- Worked as Data Scientist in DELL Technologies, Bengaluru 2013-2022
- Skillset includes COBOL, Foxpro, C/C++, Oracle, VB.NET, Bigdata, BI, Python, Julia
- Following Quantum Computing industry since Jan-2004
- Did my MCA Project title "Implementation of Quantum Computing Algorithm" in 2010
- Completed more than 7 courses on Quantum technologies in Coursera, edx, udemy
- Have hands-on experience in major Quantum Hardware and Simulators
- Building Quantum Machine Learning based solutions and R&D since 2017
- Have hands-on experience in IBM Qiskit, Xanadu Pennylane, Microsoft Q#, QuEra Bloqade, Amazon Braket, Quantinuum tket

Introduction

Quantum machine learning integrates quantum algorithms into machine learning programs.

Explores similarities between physical and learning systems, including neural networks.

Quantum computing expands hardware capabilities for machine learning.

Quantum theory provides the foundation for information processing.

Quantum bits (qubits) can represent 0, 1, or both states simultaneously (superposition).

Qubits enable parallel processing and exponential computational power.

Classical Machine Learning

Explanation of Classical Machine Learning

- foundational methods and algorithms used in the field of machine learning before the advent of deep learning techniques.

Supervised Learning:

- In supervised learning, the algorithm learns from a labeled dataset, where each example is paired with a target or outcome.
- The goal is to learn a mapping function from input variables to output variables.
- Common supervised learning tasks include regression, where the output is a continuous value, and classification, where the output is a categorical label.

Unsupervised Learning:

- Unsupervised learning involves learning patterns and structures from unlabeled data.
- The algorithm seeks to find hidden relationships or clusters within the data without explicit guidance. Clustering algorithms, such as K-Means clustering, and dimensionality reduction techniques, such as Principal Component Analysis (PCA), are examples of unsupervised learning methods.

Other Learning Paradigms:

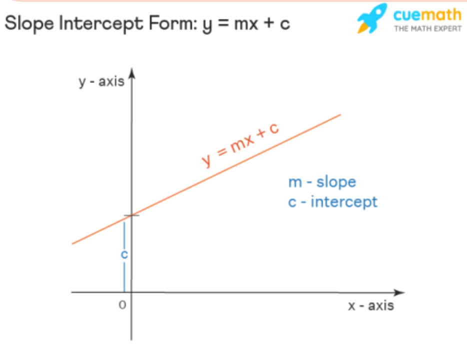
- Classical machine learning also includes semi-supervised learning, which combines elements of supervised and unsupervised learning by leveraging a small amount of labeled data along with a larger pool of unlabeled data.
- reinforcement learning, where an agent learns to make decisions by interacting with an environment and receiving rewards or penalties, is considered part of classical machine learning.

Mathematical foundation for ML

Mathematical foundation for ML

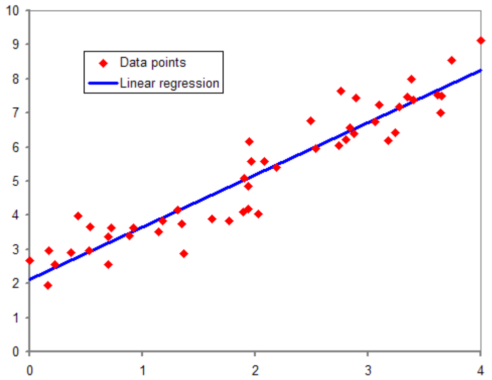
Line Equation

Y=mx+c



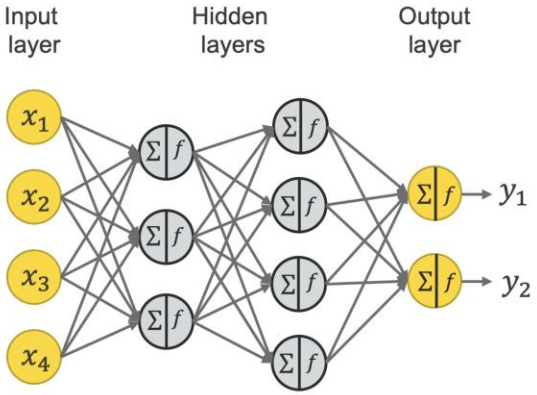
Regression

$Y=m_1x_1+m_2x_2+m_3x_3+\ldots m_nx_n+e$



Neural Networks

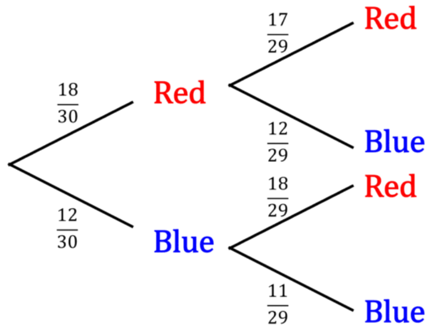
Weight and bias matrices



Random forest

Conditional probalility

P(A|B) = (P(B|A)*P(A)) / P(B)



Mathematical foundation for ML

Data fitting

- Linear regression
- Nonlinear regression

Artificial NN

- Perceptron
- FF
- RNN
- Boltzmann machine

Graphical models

- Bayesian network
- Hidden Markov model

Kernel Methods

- Kernel density estimation
- KNN
- SVM
- Gaussian process

Applications of Classical Machine Learning

Healthcare

- Predictive Analytics for Disease Diagnosis
- Personalized Treatment Recommendations
- Medical Imaging Analysis
- Drug Discovery and Development

E-commerce

- Product Recommendation Systems
- Customer Churn Prediction
- Price Optimization
- Inventory Management

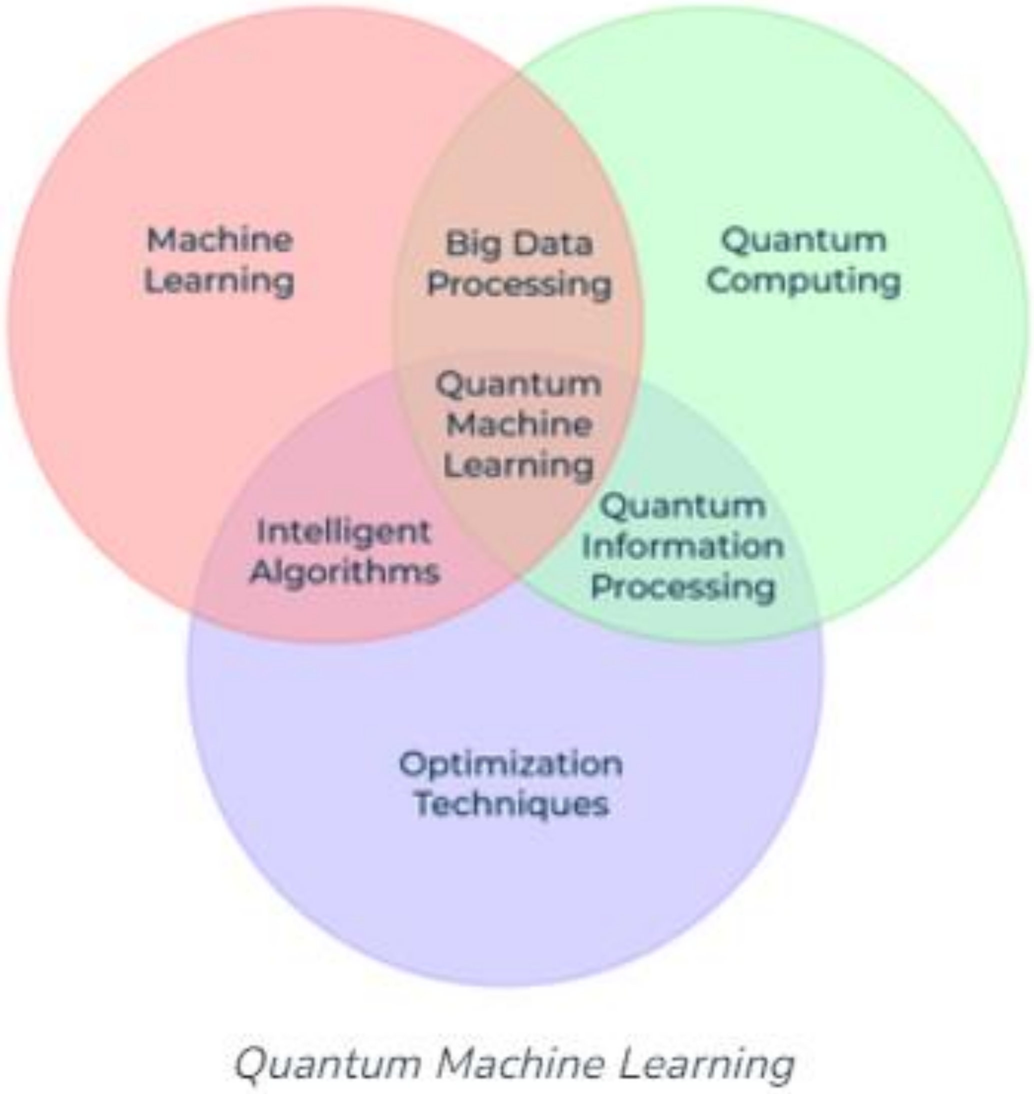
Finance

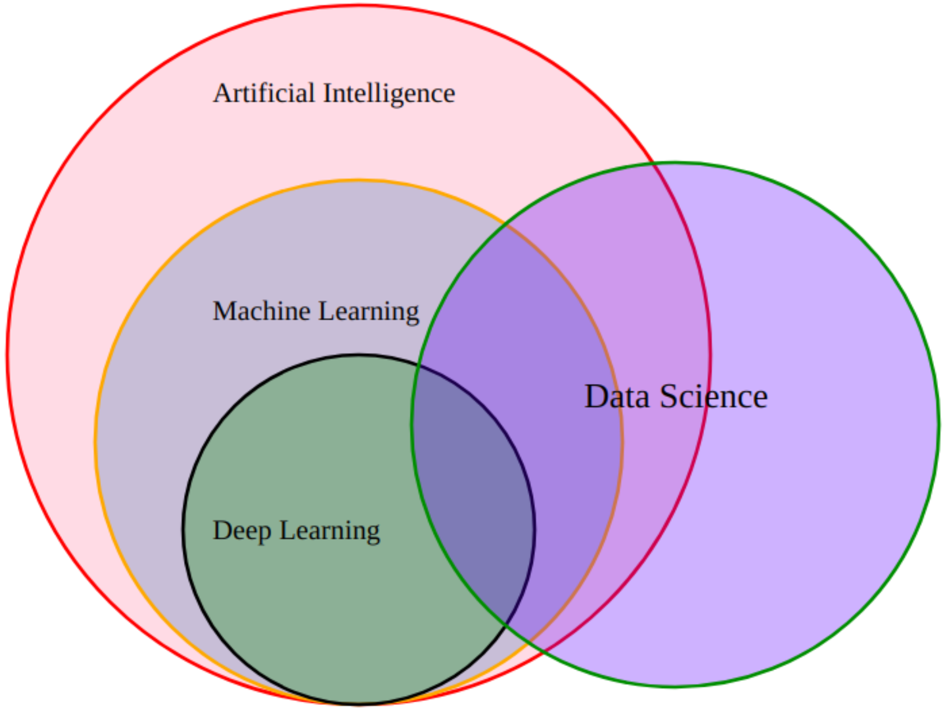
- Fraud Detection
- Risk Assessment and Management
- Algorithmic Trading
- Customer Segmentation and Personalization

Marketing

- Customer Segmentation
- Sentiment Analysis
- Predictive Modeling for Campaign Optimization
- Dynamic Pricing

Venn Diagram of QML





https://www.researchgate.net/figure/Venn-Diagram-for-AI-ML-NLP-DL_fig1_353939315

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Benefits of QML

Potential for significant speedups

Access to new possibilities

Development of new algorithms

Speed

- Certain NP hard problems can be solved in Polynomial time

Accuracy

- Quantum algorithms can process information without approximation

Security

- Quantum Cryptography and Quantum Communication will ensure that our data and QML models are secure from hackers

Scalability

- As the number of qubits are increasing, quantum computers can process large volume of data exponentially compared to classical computers

Novel Application

- Optimizing quantum circuits, financial portfolio and other optimization problems

Challenges of QML

Quantum computers are still in their early stages

Quantum algorithms can be complex to design and implement

The field is young and rapidly evolving, requiring continuous learning and adaptation

Getting Started with QML

Learn the basics of quantum mechanics

Explore online resources

Experiment with QML platforms

Follow the latest developments

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QML vs Classical ML

Aspect	Quantum Machine Learning (QML)	Classical Machine Learning (CML)
Computation Speed	Potentially faster for specific problems due to quantum parallelism and entanglement	Generally slower for certain complex problems, especially those involving high-dimensional data
Dimensionality Handling	Capable of handling exponentially larger feature spaces efficiently	Limited by classical computational resources; struggles with very high-dimensional data
Algorithm Complexity	Complex algorithms that require deep understanding of quantum mechanics	Well-established algorithms with extensive libraries and support
Error Rates	High error rates due to quantum decoherence and noise in current quantum hardware	Low error rates in mature classical hardware; robust error correction techniques available
Scalability	Currently limited by the number of qubits and coherence time; ongoing research to scale up	Highly scalable with the ability to handle large datasets using distributed computing
Implementation	Requires specialized quantum hardware which is currently expensive and not widely available	Can be implemented on standard classical computers, from desktops to large-scale clusters
Practical Applications	Promising in fields like cryptography, optimization, and certain types of machine learning problems	Widely applied across various domains such as image recognition, natural language processing, and predictive analytics
Research and Development	Rapidly evolving field with significant breakthroughs anticipated in the near future	Established field with a vast amount of existing research and continuous incremental improvements
Energy Efficiency	Potentially more energy-efficient for certain computations due to quantum advantages	Generally requires significant computational power, especially for large-scale data processing
Educational Resources	Limited educational resources and fewer experts in the field currently	Extensive educational resources and a large community of practitioners and researchers

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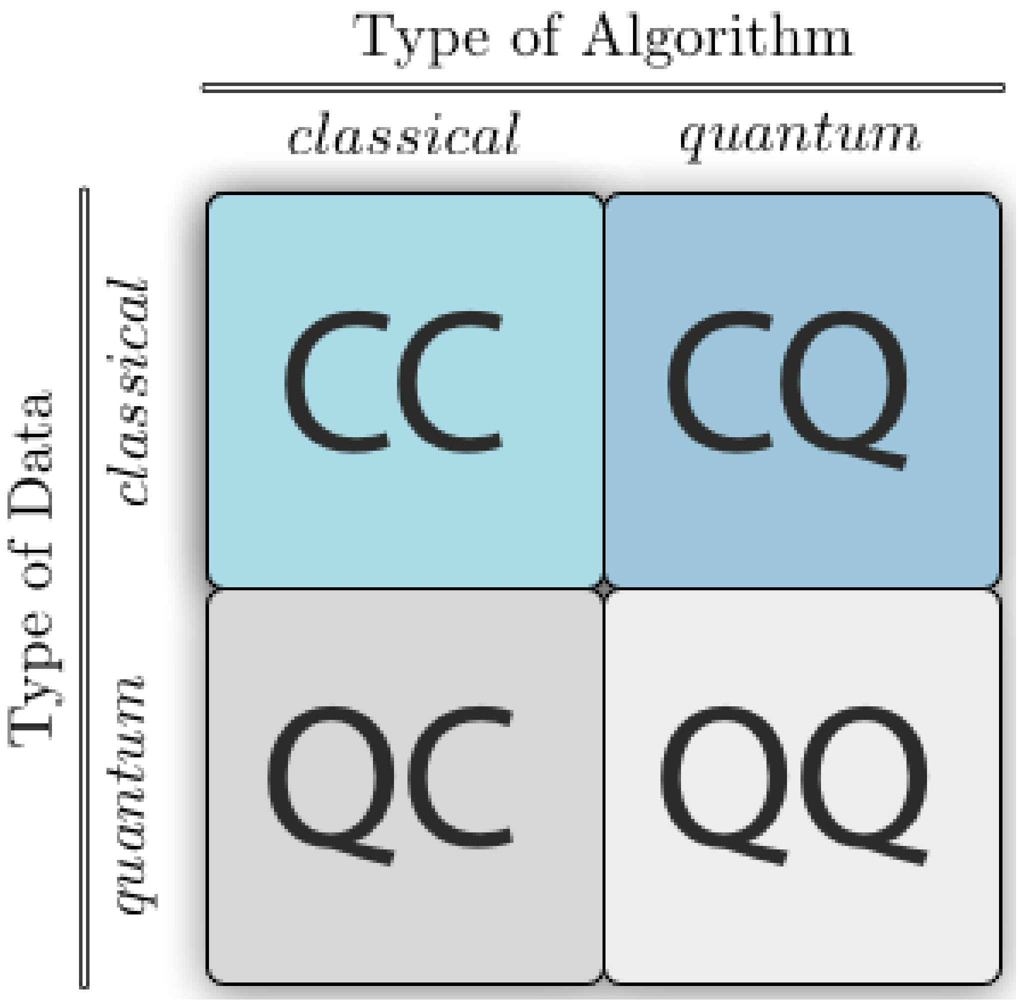
Four approaches to QML



https://commons.wikimedia.org/wiki/File:Qml_approaches.svg
https://fastercapital.com/content/Quantum-Machine-Learning--Enhancing-AI-with-QIP.html

Four approaches to QML

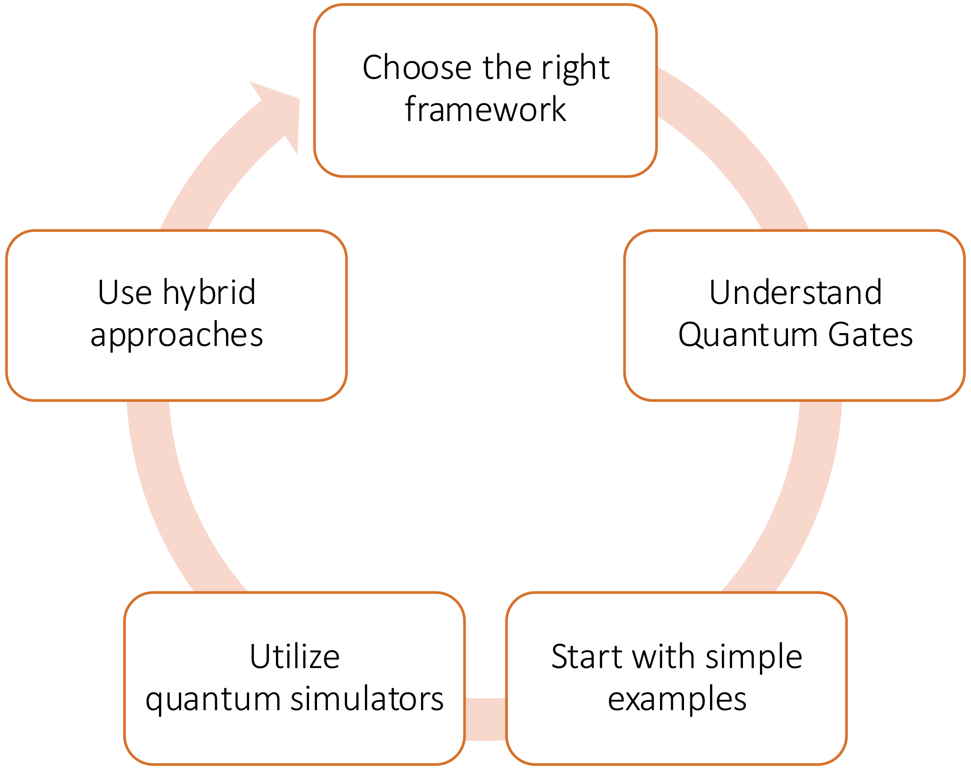
Four approaches to QML

Classical-Classical (QML)
- both data and computation remain classical
- algorithms are inspired by quantum principles

Quantum-Classical (Hybrid QML)
- combines classical data preprocessing with quantum computations for specific tasks
- classical algorithms prepare and analyze data

Classical-Quantum (Quantum-Enhanced Machine Learning)
- quantum resources are used to enhance specific steps within classical machine learning algorithms
- features extraction, representation learning, or model training.

Quantum-Quantum (Full Quantum Machine Learning)
- qubits encode and process information, and quantum algorithms tackle the entire machine learning problem



https://fastercapital.com/content/Quantum-Machine-Learning--Enhancing-AI-with-QIP.html#Implementing-QML-in-practice

Quantum Information Encoding

allows representing classical information in the intricate language of quantum bits (qubits)

- Variational Quantum Eigensolvers (VQE)
- Quantum Approximate Optimization Algorithms (QAOA)
- Quantum Neural Networks
- Gottesman-Kitaev-Preskill (GKP) encoding
- Error correction capabilities

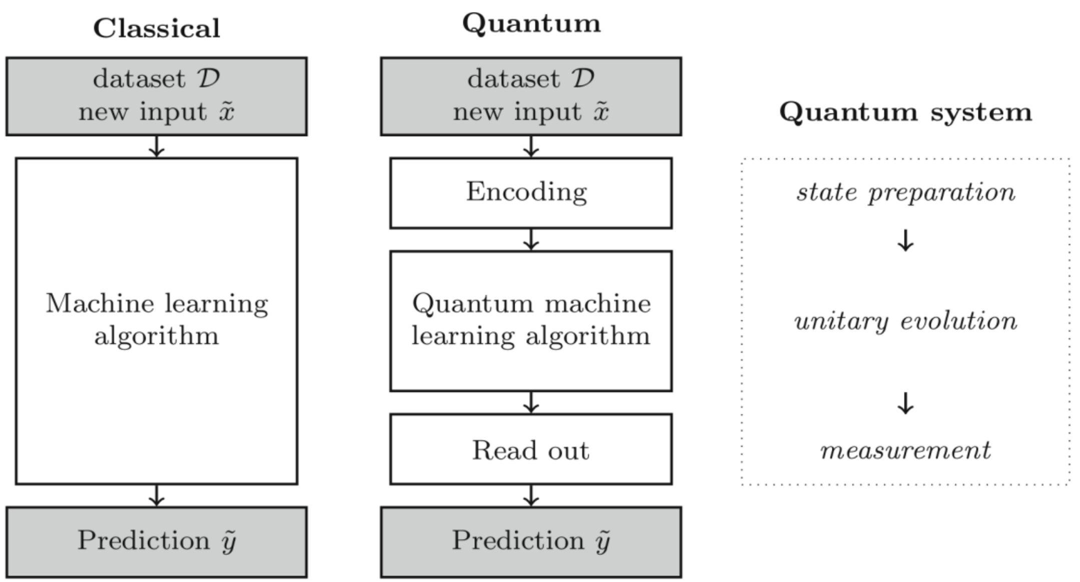


Fig. 5.1 In order to solve supervised machine learning tasks based on classical datasets, the quantum algorithm requires an information encoding and read out step that are in general highly non-trivial procedures, and it is important to consider them in the runtime. Adapted from [2]

Table 5.1 Comparison of the four encoding strategies for a dataset of M inputs with N features each. While basis, amplitude and Hamiltonian encoding aim at representing a full data set by the quantum system, qsample encoding works a little different in that it represents a probability distribution over random variables. It therefore does not have a dependency on the number of inputs M. **Only certain datasets or models can be encoded in this time. See text for details.*

Encoding	Number of qubits	Runtime of state prep	Input features
Basis	N	$\mathcal{O}(MN)$	Binary
Amplitude	$\log N$	$\mathcal{O}(MN)/\mathcal{O}(\log(MN))$*	Continuous
Qsample	N	$\mathcal{O}(2^N)/\mathcal{O}(N)$*	Binary
Hamiltonian	$\log N$	$\mathcal{O}(MN)/\mathcal{O}(\log(MN))$*	Continuous

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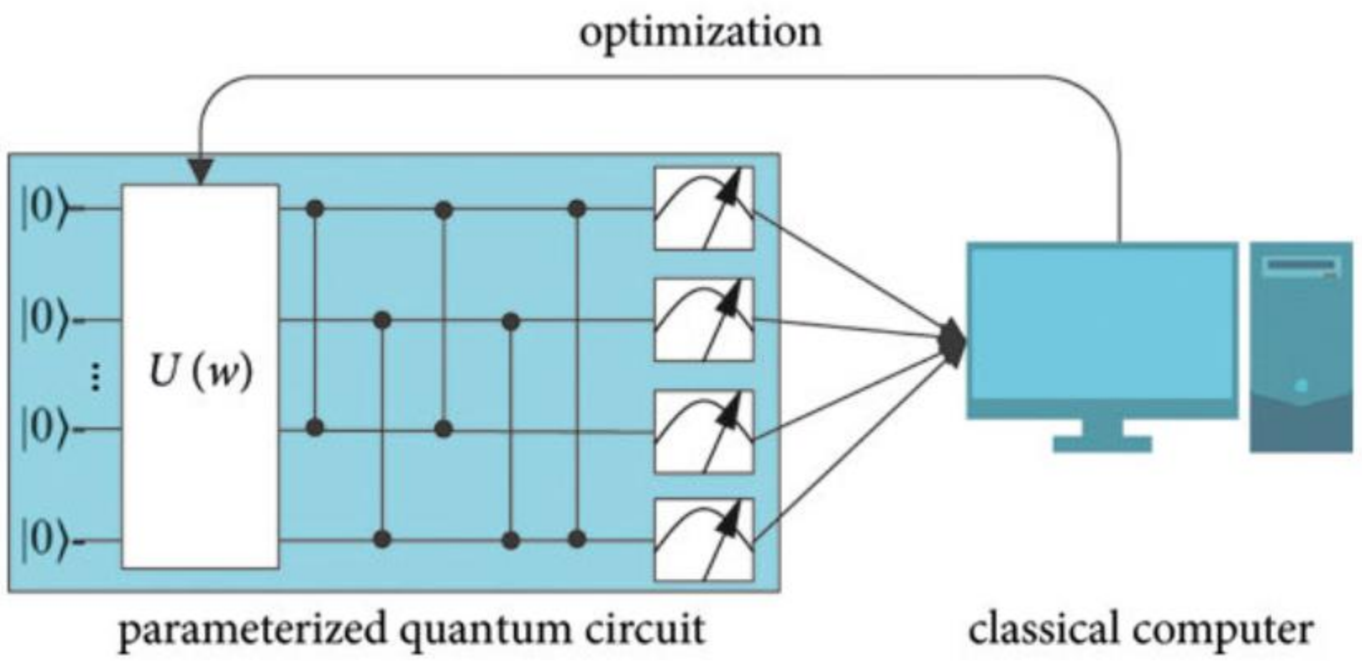
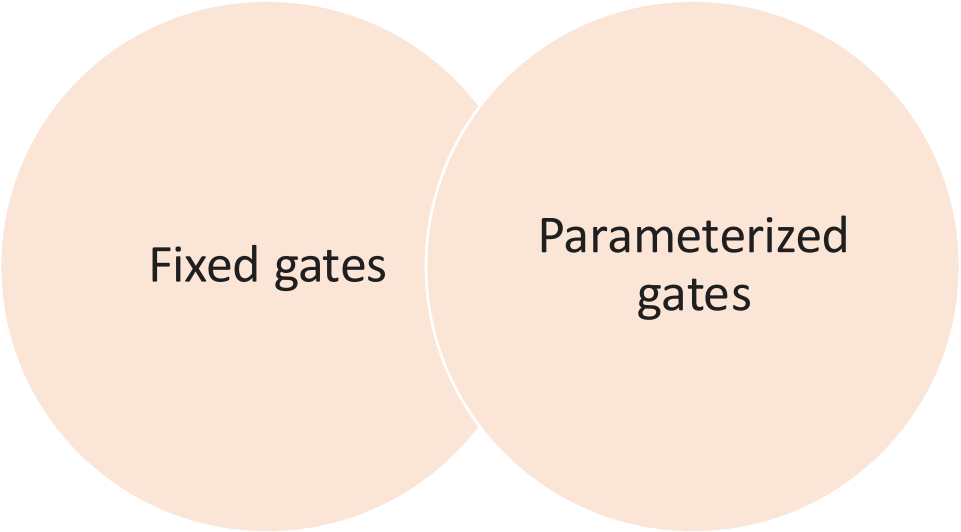
Parameterized quantum circuits (PQC)





PQCs offer several advantages

Universality

Learning potential

Expressivity

Applications of PQCs

Variational Quantum Eigensolvers (VQE)

Quantum Approximate Optimization Algorithms (QAOA)

Generative quantum models

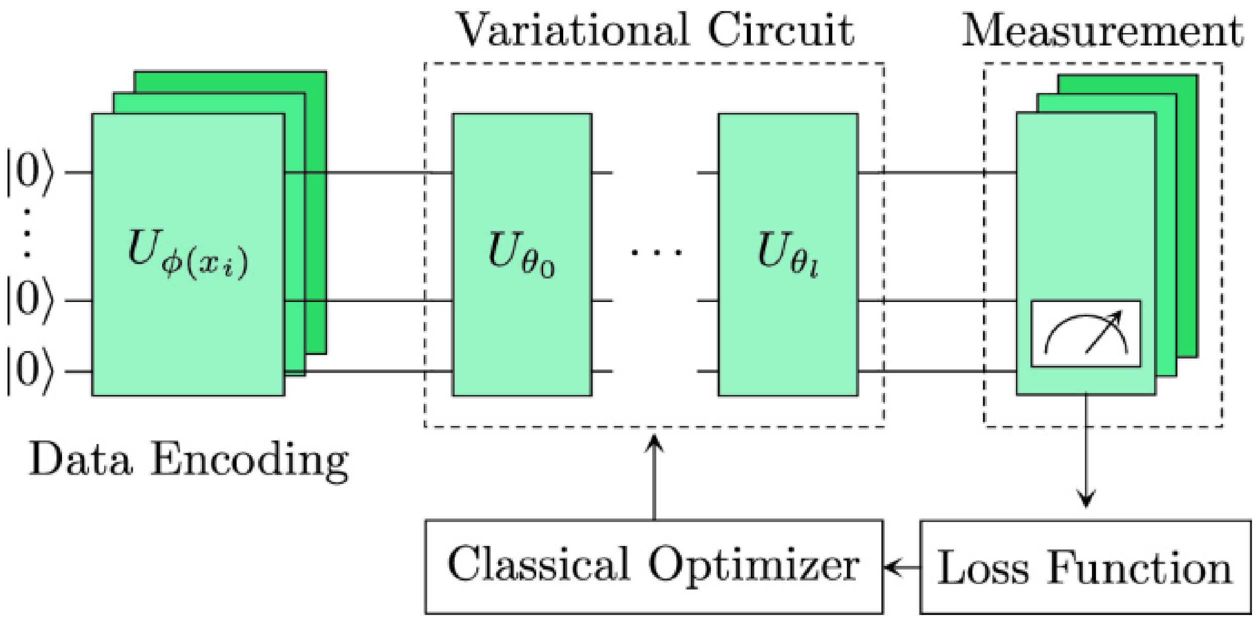
Challenges and considerations

Finding optimal parameters

Limited by current hardware

Theoretical understanding

Training parameterized quantum circuits



Solve optimization problems

Classify data

Generate new data

Hybrid process involving both the quantum and classical worlds

Encode data

↓

Variational circuit

↓

Measurement

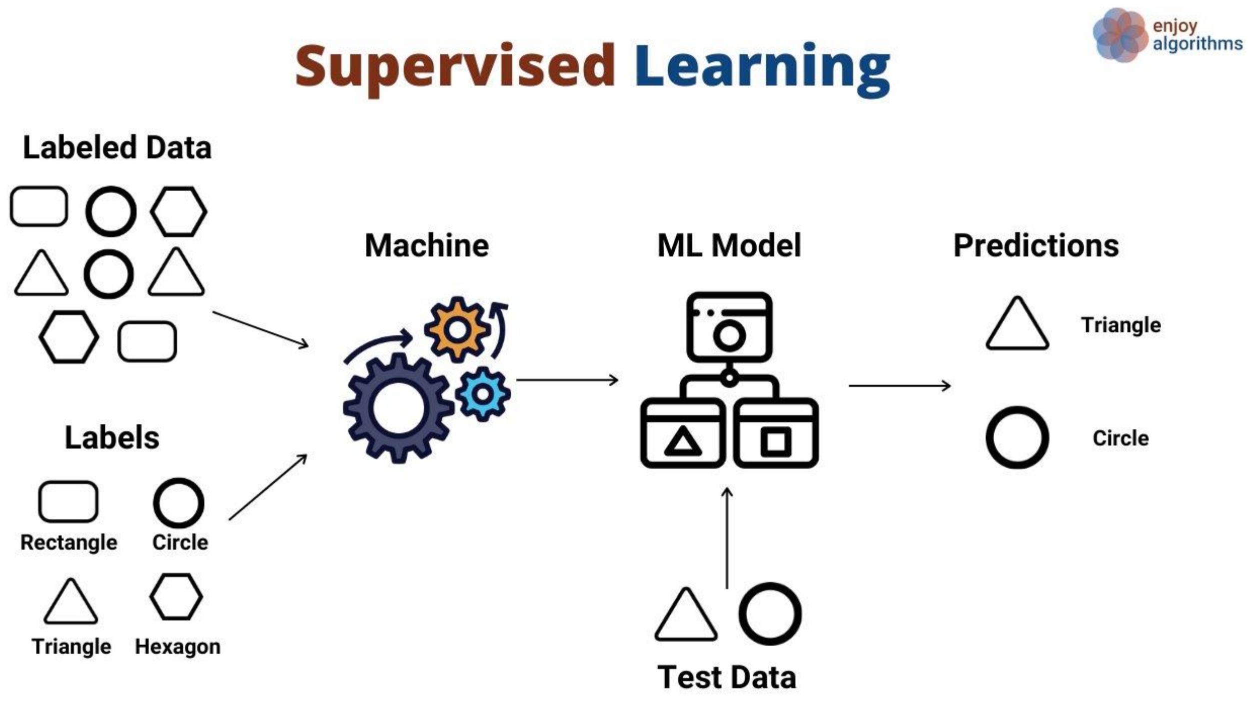
↓

Optimization

↓

Repeat: Steps 2-5

Supervised Learning



Supervised learning is a common approach where algorithms learn from labeled data to make predictions or classifications.

- Preparing labeled data
- Training the circuit
- Evaluation

Advantages of using PQCs for supervised learning

- **Potential for improved performance**
- **Flexibility**

Quantum variational classification

supervised learning using parameterized quantum circuits.

Comparison to classical approaches:

Potential advantages

Feature extraction:

- Quantum circuits can exploit quantum phenomena like entanglement for more efficient feature extraction, potentially leading to better classification performance.

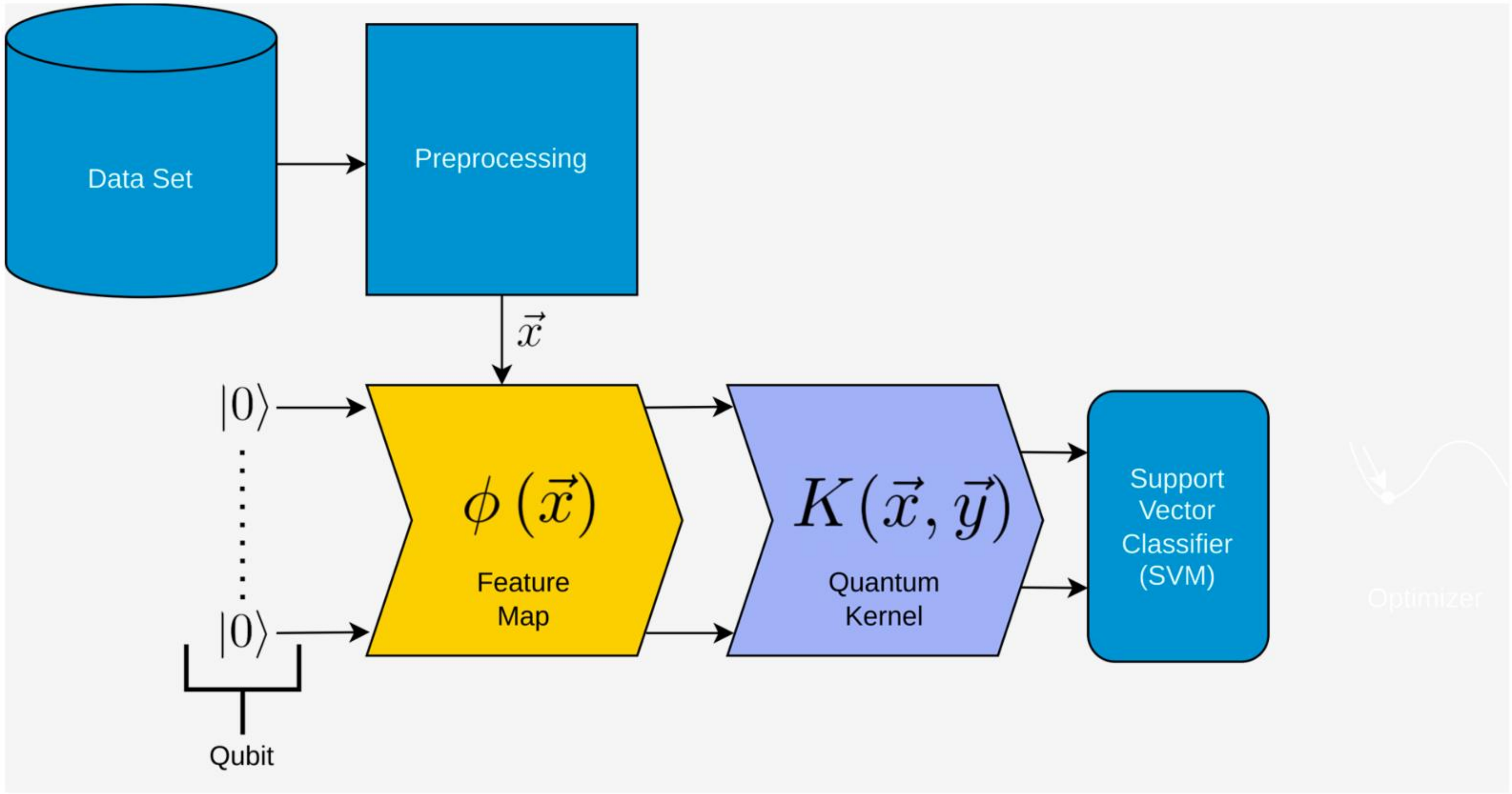
Representation of complex data:

- QVC can inherently handle high-dimensional data, overcoming limitations of classical feature engineering.

Applications:

Image classification:	Financial analysis:	Drug discovery:	Materials science:
• Identifying objects in images with potentially higher accuracy than classical methods.	• Predicting market trends or detecting fraud more effectively.	• Designing new drugs by simulating molecules and their interactions.	• Discovering new materials with desired properties through quantum property prediction.

Quantum kernel estimation



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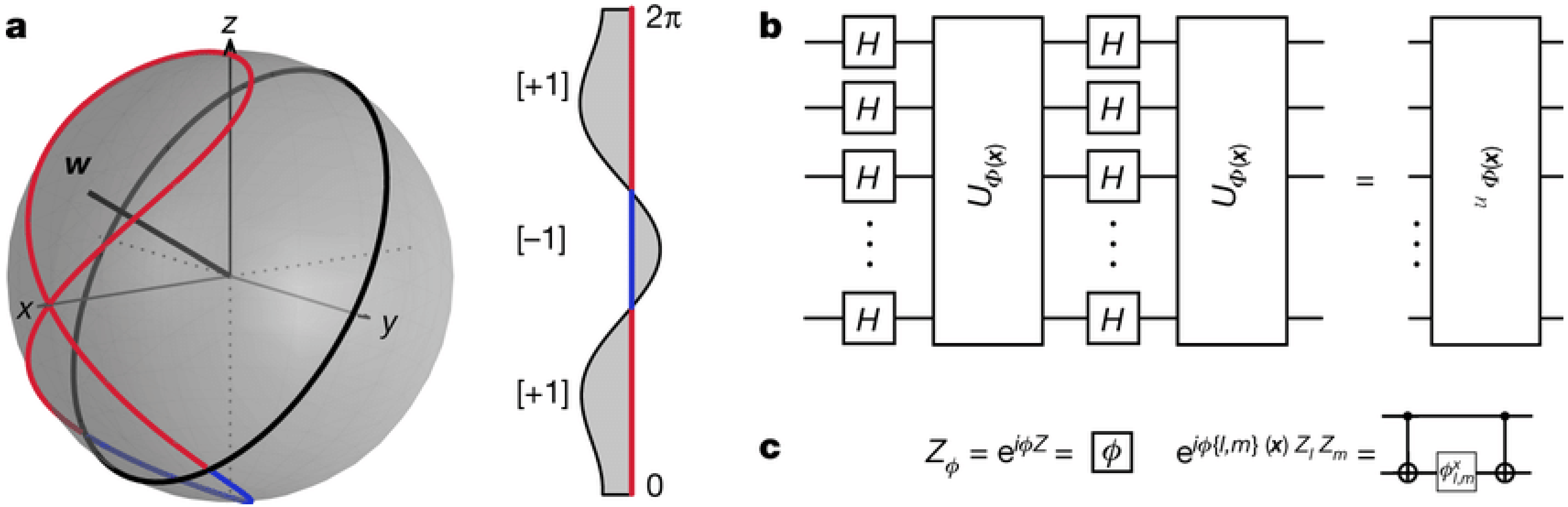
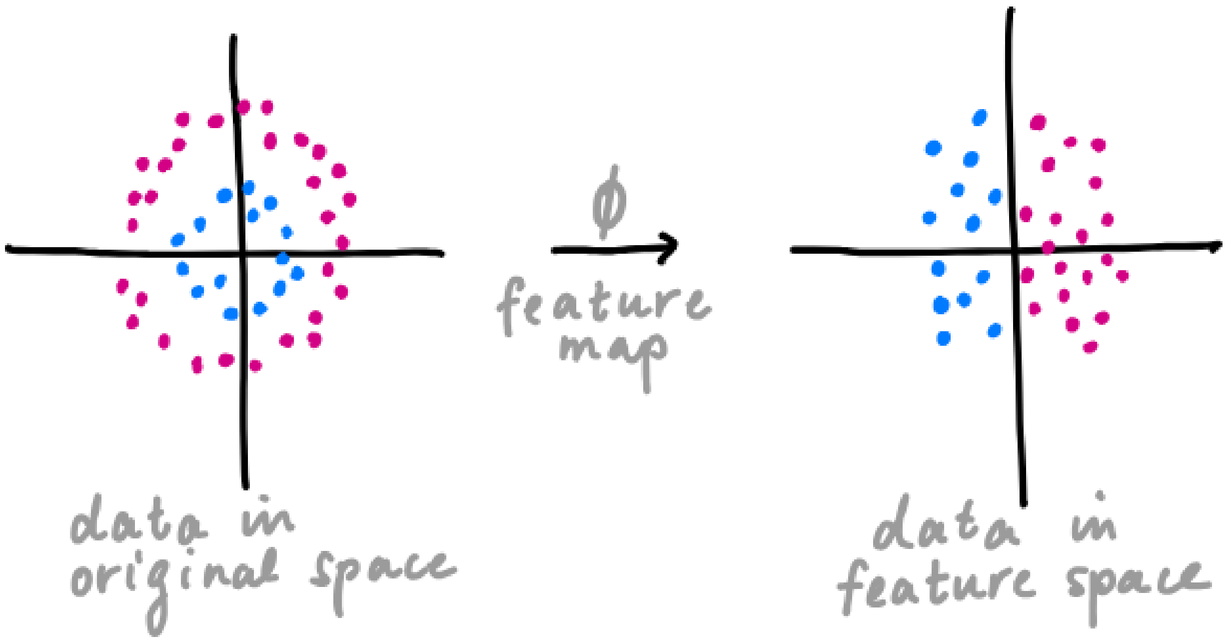
Quantum feature map and kernels



fundamental component of quantum machine learning algorithms, particularly those that involve kernel-based methods.



Quantum Feature Map:

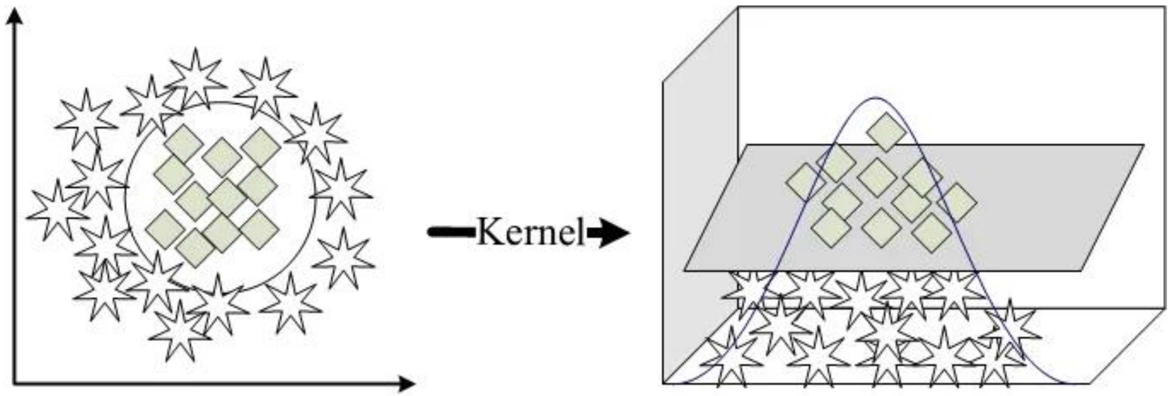
- A quantum feature map is a quantum circuit that encodes classical data points into quantum states.

Kernel Computation

Once the data has been encoded into quantum states using the quantum feature map, the next step is to compute the kernel matrix.

The kernel matrix represents the pairwise inner products or similarities between pairs of data points in the high-dimensional feature space induced by the quantum feature map.

The kernel matrix is computed using quantum algorithms or quantum-inspired techniques that exploit the quantum representation of the data.



Linealy inseparable

Linearly separable

Quantum Support Vector classification (QSVM)

A fascinating approach that builds upon the foundation of both classical Support Vector Machines (SVMs) and the power of quantum computing.

How does it work?

Data encoding

Quantum kernel computation

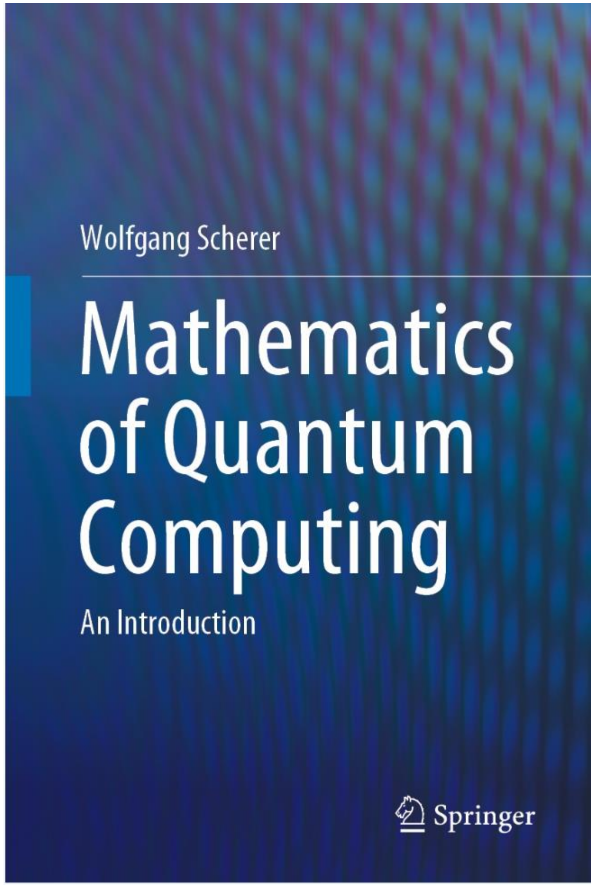
SVM algorithm

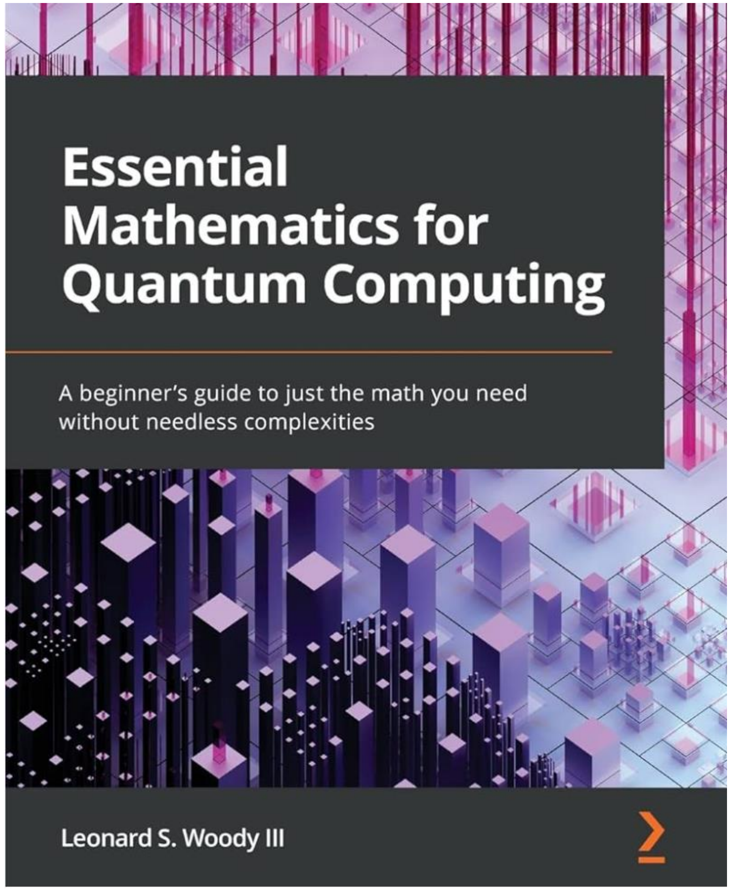
Advantages

Potential for better performance

Handling high-dimensional data

Recommended resources





Linear Algebra - Full College Course from freecodecamp.org
https://www.youtube.com/watch?v=JnTa9XtvmfI

Linear Algebra – Gilbert Strang
https://www.youtube.com/watch?v=7UJ4CFRGd-U&list=PL221E2BBF13BECF6C

3Blue1Brown
https://www.youtube.com/c/3blue1brown

Veritasium
https://www.youtube.com/playlist?list=PLkahZjV5wKe-Z1RP3ZiYwe8JSAolmqF9M

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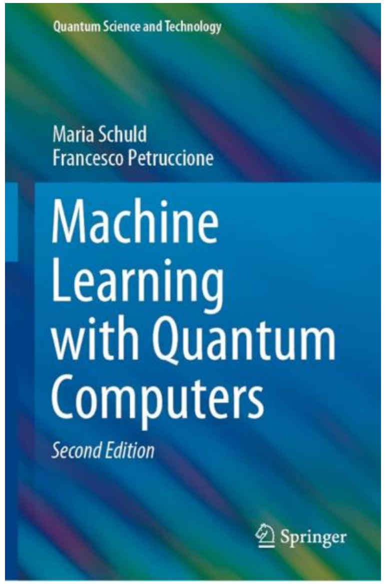
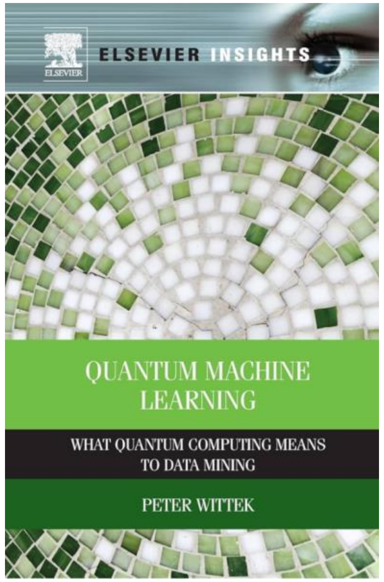
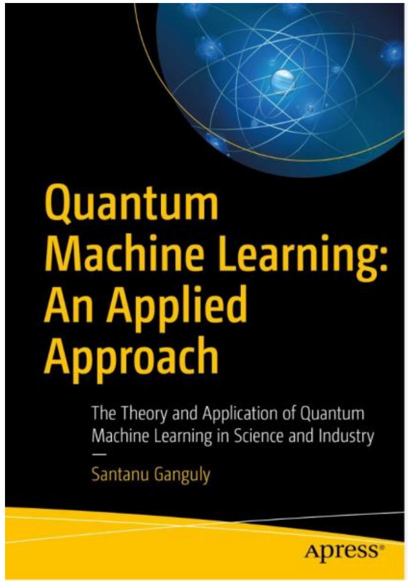
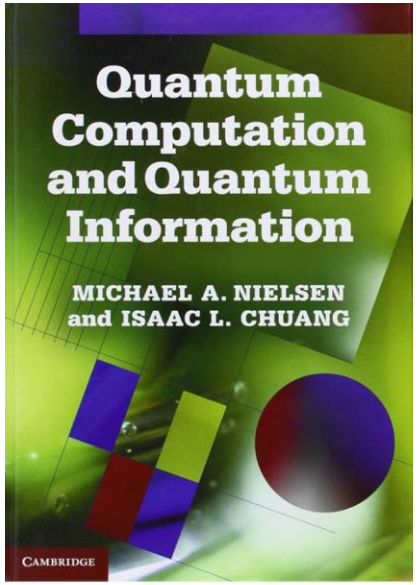
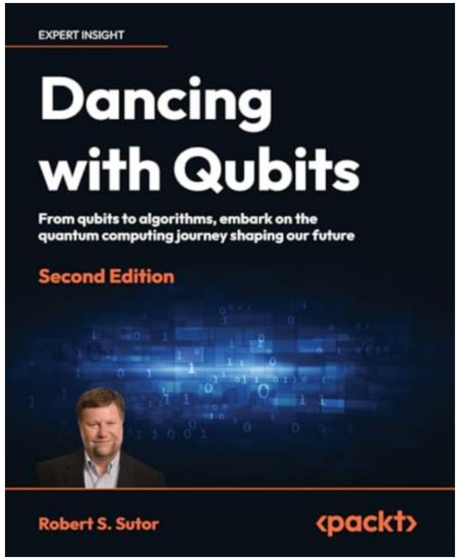
Recommended resources

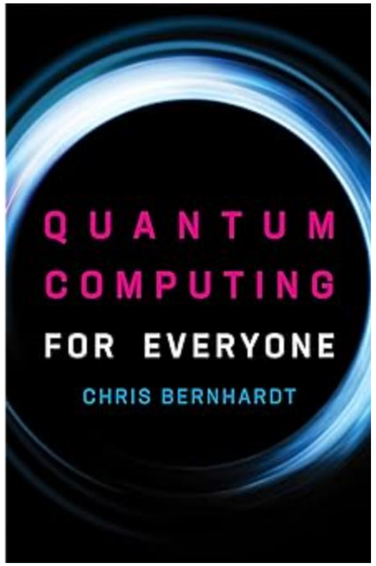


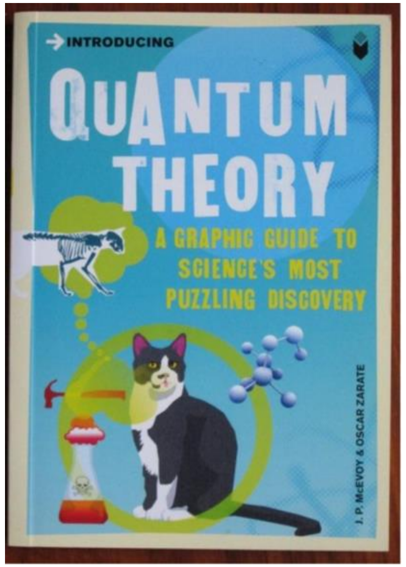












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Books & Resources

Quantum Machine Learning: What Quantum Computing Means to Data Mining

- Peter Wittek

Quantum Machine Learning

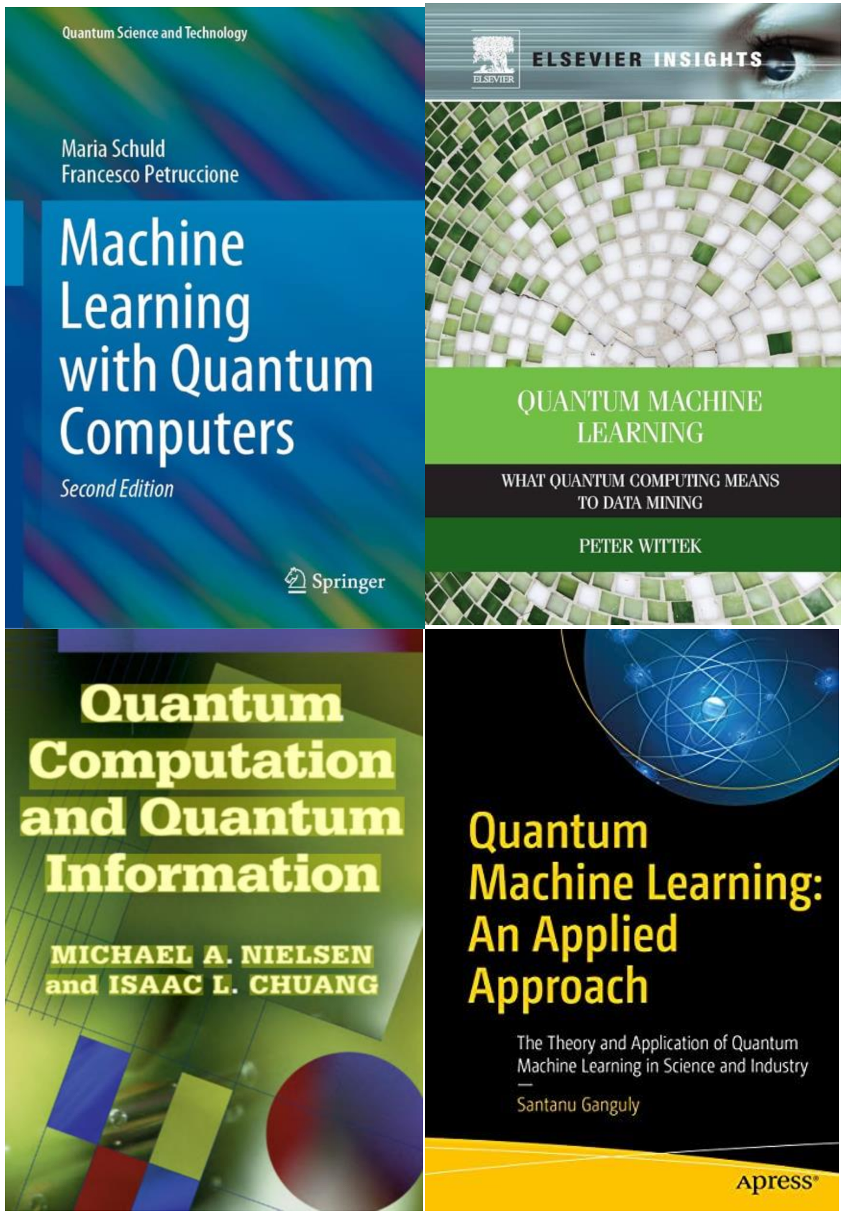
- Maria Schuld and Francesco Petruccione

Quantum Machine Learning: An Applied Approach

- Santanu Ganguly

Quantum Computation and Quantum Information

- Michael A. Nielsen and Isaac L. Chuang



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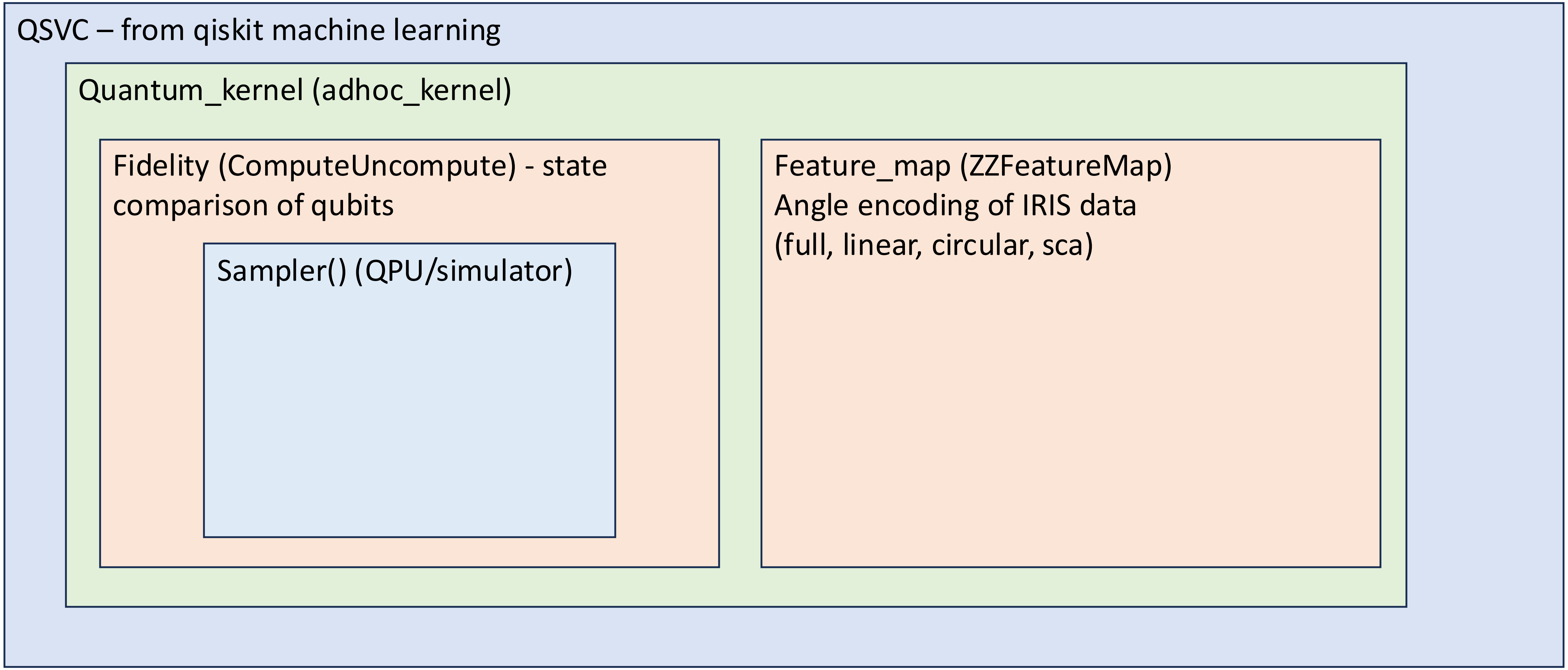
How to Build Quantum Programs?

- IBM Quantum Composer (Learning, Proof of Concept)
- Google Colab (PoC, Collaborative dev)
  - Pip install everytime in a new notebook
- Jupyter notebook in localhost
  - Virtual environment is highly recommended
- VSCode and .py in localhost (Production systems)
  - Virtual environment is highly recommended

Important frameworks

- Qiskit Ecosystem
  - https://www.ibm.com/quantum/ecosystem
- Pennylane.ai
  - https://pennylane.ai/qml/demonstrations
- Qiskit Machine Learning
  - https://qiskit-community.github.io/qiskit-machine-learning/index.html
- QuEra Bloqade
  - https://github.com/QuEraComputing/bloqade-python
- Quantinuum Lambeq for QNLp
  - https://docs.quantinuum.com/lambeq/index.html

QSVM Demo


QSVC – from qiskit machine learning
Quantum_kernel (adhoc_kernel)
Fidelity (ComputeUncompute) - state comparison of qubits
Sampler() (QPU/simulator)
Feature_map (ZZFeatureMap)
Angle encoding of IRIS data
(full, linear, circular, sca)