

Focused Tutorial on Quantum Computing

TBD

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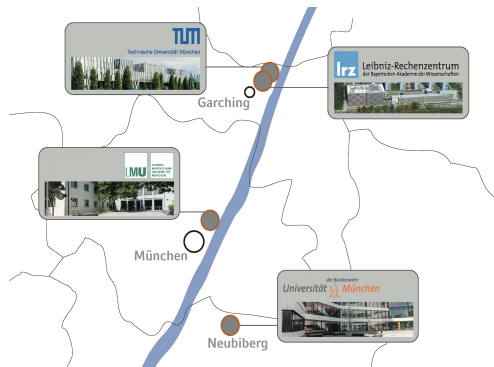
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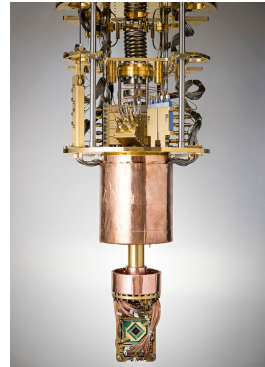


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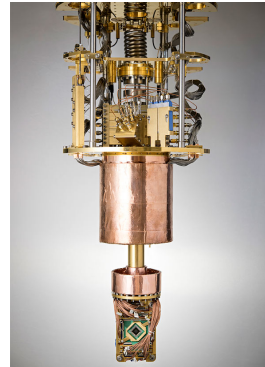
What is Quantum Computing?

- Exploiting quantum mechanical effects for computations



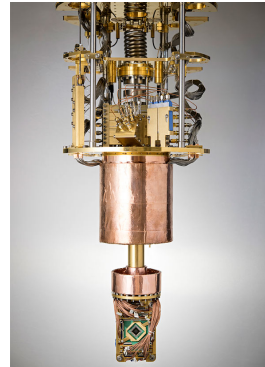
What is Quantum Computing?

- Exploiting quantum mechanical effects for computations
 - Superposition



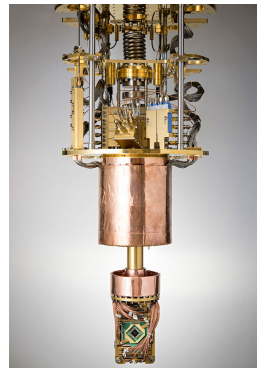
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 - Interference



What is Quantum Computing?

- Exploiting quantum mechanical effects for computations
 - Superposition
 - Interference
- Optimal hardware yet to be determined



Why do we need Quantum Computing?

- Speed up classical computation

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- Speed up classical computation
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 - Bug-proof communication
 - True randomness

Outlook of today's tutorial

- First part: Introduction to mathematics of QC
 - Qubit states
 - State manipulation via unitary matrices
 - Quantum circuits
- Second part (after LRZ site visit): Classification with quantum computing
 - Quantum programming in PennyLane framework
 - Variational quantum circuits
 - Binary classification

Classical vs. Quantum Computing

	Classical Computing	Quantum Computing
Basic States	Either 0 or 1	Superposition of 0 and 1
Operations	Logic (boolean) gates	Unitary reversible gates
Copying States	Yes	No
Readout	No information loss	Superposition is destroyed; information loss

Qubit States I

- State: Qubit – 0, 1 or a *superposition* of 0 and 1

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- Represented by a two-dimensional *normalized* vector:

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \alpha, \beta \in \mathbb{C}$$

where

$$|\alpha|^2 + |\beta|^2 = 1$$

Qubit States II

- Instead of vectors, a qubit state can also be written in the *Dirac Notation*:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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Then we can write

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad \alpha, \beta \in \mathbb{C}$$

instead of

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \alpha, \beta \in \mathbb{C}$$

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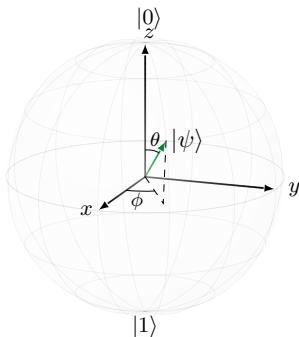
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$$\langle \psi| = \alpha^* \langle 0| + \beta^* \langle 1| \quad \alpha, \beta \in \mathbb{C}$$

Bloch Sphere

We can interpret a single qubit vector as a point on a three dimensional plane:



$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi} |1\rangle$$

Unitary Operations

- Quantum operations represented by quantum gates
- The length of the state vector must remain $|\alpha|^2 + |\beta|^2 = 1$

→ Requires unitary matrix operations on the state vector.


$$\begin{pmatrix} u_{00} & u_{10} \\ u_{01} & u_{11} \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} u_{00} \cdot \alpha + u_{10} \cdot \beta \\ u_{01} \cdot \alpha + u_{11} \cdot \beta \end{pmatrix}$$

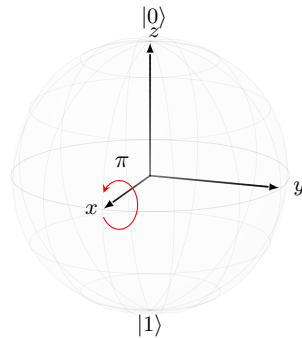
- We can represent operations on qubits in the quantum circuit model:

$$|\psi\rangle \text{ --- } \boxed{U} \text{ --- } |\psi'\rangle$$

Single Qubit Gates I


Pauli matrices:


▪ $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ 

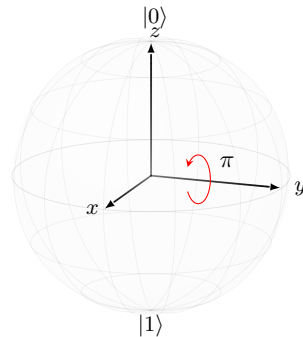


Single Qubit Gates I

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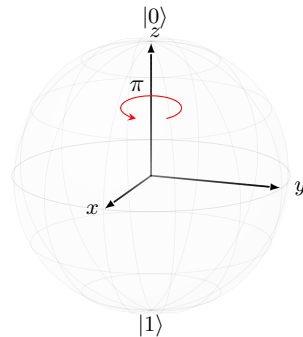
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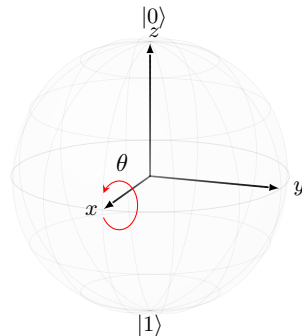
▪ $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ —  —



Arbitrary Rotations

$R_\gamma(\theta)$ -Gate: Rotation by θ around the X/Y/Z axis (?: X, Y, or Z)

$$\blacksquare R_x(\theta) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -i \sin(\frac{\theta}{2}) \\ -i \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix} \quad \text{---} \boxed{R_x(\theta)} \text{---}$$

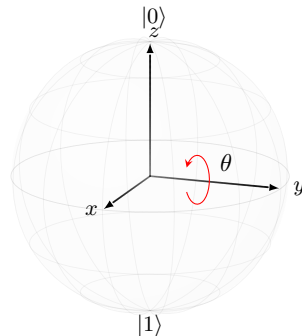


Arbitrary Rotations

$R_\theta(\theta)$ -Gate: Rotation by θ around the X/Y/Z axis (?: X, Y, or Z)

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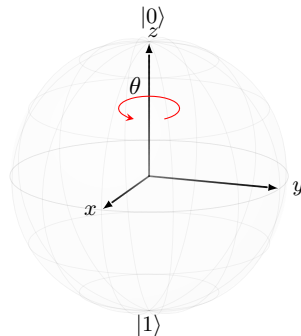
Arbitrary Rotations

$R_{\hat{n}}(\theta)$ -Gate: Rotation by θ around the X/Y/Z axis (?: X, Y, or Z)

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$$\blacksquare R_z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} \text{---} \boxed{R_z(\theta)} \text{---}$$



Measurement I

Given the qubit in the state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is measured. Then...

... the probability of measuring $|0\rangle$ is $|\alpha|^2$

... the probability of measuring $|1\rangle$ is $|\beta|^2$

Probability of measuring $|0\rangle$ for state $|\psi\rangle = H|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$:

$$P(|0\rangle) = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}$$

Measurement II

- We cannot read the state of a qubit, we can only measure the qubit
 - With a measurement on a qubit, its state collapses to one of the basis states
 - The original quantum state cannot be restored anymore
- We have to measure multiple times to approximate the original quantum state

Quantum Registers

- Multiple qubits can be combined to a *quantum register* by calculating their tensorproduct:

$$\begin{pmatrix} \alpha_{n-1} \\ \beta_{n-1} \end{pmatrix} \otimes \begin{pmatrix} \alpha_{n-2} \\ \beta_{n-2} \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix}$$

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- Quantum operations on quantum registers are represented by the tensorproduct of the corresponding matrices (dimension: $2^n \times 2^n$)

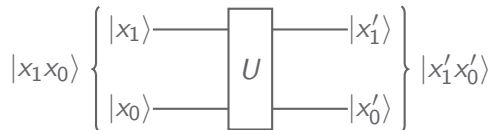
Two Qubit Register

$$|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle$$

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

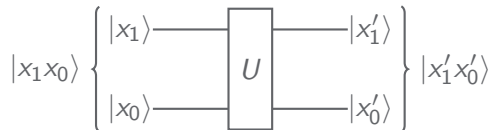
Multi-Qubit Gates

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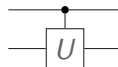
For instance, we can combine the existing single qubit gates using the tensor product:

$$X \otimes X =$$

Controlled Qubit Operations

- An operation on a qubit may depend on the state of another qubit → Any single-qubit gate can have a “controlled version”

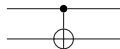
$$CU = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{10} \\ 0 & 0 & u_{01} & u_{11} \end{pmatrix}$$



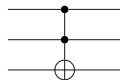
Controlled Qubit Operations

- An operation on a qubit may depend on the state of another qubit → Any single-qubit gate can have a “controlled version”
- Most common: CX/CNOT and CCX/CCNOT/Toffoli Gate

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



$$CCX = \begin{pmatrix} & & & 0 & 0 \\ & & & \vdots & \vdots \\ & \mathbb{I}_6 & & 0 & 0 \\ 0 & \dots & 0 & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$



The SWAP Operation

- The SWAP operation “swaps” the states of two qubits:

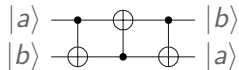
$$\text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{array}{c} |a\rangle \text{ --- } \times \text{ --- } |b\rangle \\ |b\rangle \text{ --- } \times \text{ --- } |a\rangle \end{array}$$

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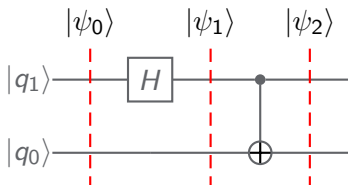
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- It can be implemented with three CNOT gates:



Entanglement I

By applying a controlled gate (e.g., CNOT) on qubits in superposition we can create entanglement:
e.g., $|q_1 q_0\rangle = |00\rangle$:



$$|\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

\Rightarrow We either measure both qubits in $|0\rangle$ **or** in $|1\rangle$.

Entanglement II

Definition

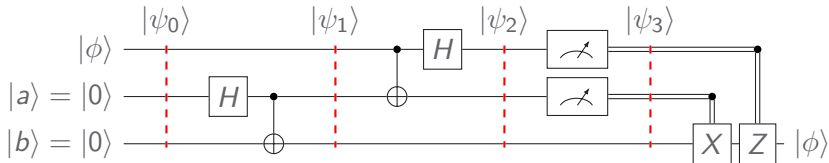
Qubits are *entangled* with each other iff the qubit state cannot be represented as a tensor product of single qubit states.

$$\text{e.g., } \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

No-Cloning Theorem

- Entanglement is **not** equivalent to cloning a qubit state
- It is not possible to clone or copy an arbitrary qubit state
- With entanglement, it is possible to teleport an arbitrary state from one qubit to another

Teleportation



Observables

- Hermitian operators that describe quantum-physical characteristics of a system

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- The expectation value is calculated with respect to the eigenvalues of the observable, not the measurement bases

Pauli-Z Matrix as Observable

- Z matrix: $Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
- The expectation value can be calculated with $\langle \psi | Z | \psi \rangle$
- Examples:
 1. $\langle 0 | Z | 0 \rangle =$
 2. $\langle 1 | Z | 1 \rangle =$
 3. $\frac{1}{\sqrt{2}}(\langle 0 | + \langle 1 |) \cdot Z \cdot \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) =$

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- Near-term goal: design quantum circuits/algorithms that...

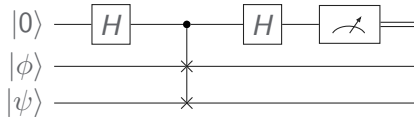
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- Near-term quantum algorithms: Variational Quantum Algorithms (VQAs)

Swap Test I

Means to measure the distance d of two quantum states $|\phi\rangle$ and $|\psi\rangle$
 $d = |\langle\psi|\phi\rangle|^2$ (angle² between $|\psi\rangle$ and $|\phi\rangle$)



Swap Test II

- At the end of the circuit the probability of measuring $|0\rangle$ is the following

$$P(\text{"Measure } |0\rangle \text{ "}) = \frac{1}{2} + \frac{1}{2} |\langle \psi | \phi \rangle|^2$$

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- If $|\psi\rangle$ and $|\phi\rangle$ are orthogonal ($|\langle \psi | \phi \rangle|^2 = 0$), then $P(\text{"Measure } |0\rangle \text{"}) = \frac{1}{2}$
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- Then $d = |\langle \psi | \phi \rangle|^2 = 2P(\text{"Measure } |0\rangle \text{"}) - 1$

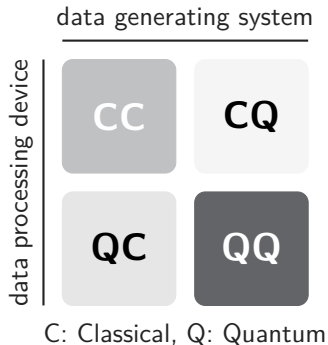
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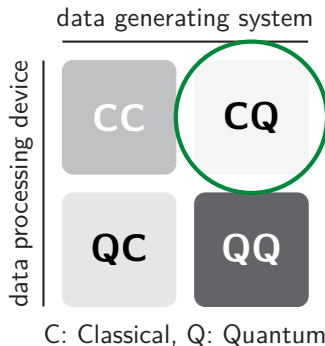
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- Then $d = |\langle \psi | \phi \rangle|^2 = 2P(\text{"Measure } |0\rangle \text{ "}) - 1$
- With multiple repetitions of the SWAP test, the distance d can be approximated with any precision

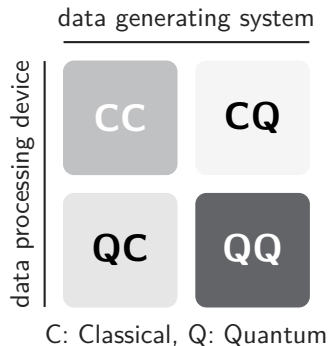
Overview



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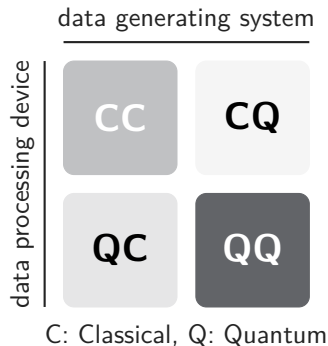
Overview – Classical Machine Learning



1. Input

- Training data X_{train}
- Initial parameter vector θ

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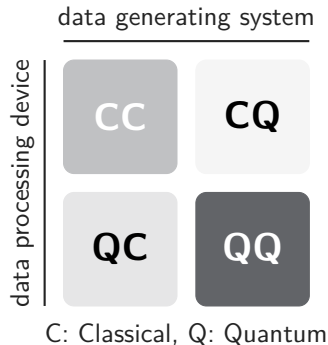


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2. Model: $f(X_{\text{train}}, \theta) = \hat{y}$

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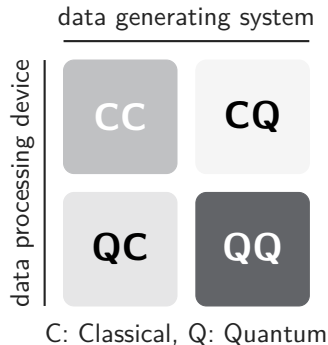
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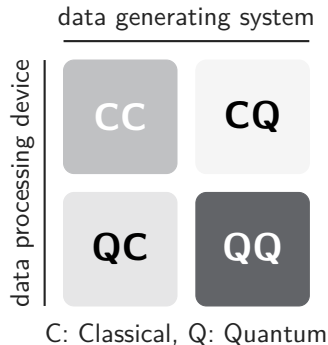
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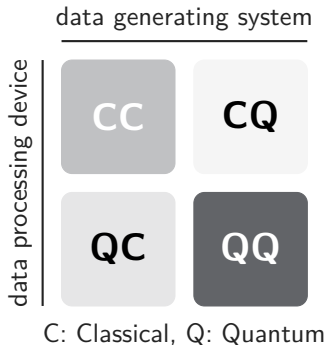
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3. Prediction: Score with cost function $C(\hat{y}, y)$
4. Update θ based on gradient-based techniques

Overview – Classical Machine Learning



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5. Repeat starting from step 2

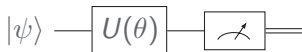
Overview – Classical Machine Learning



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Classical Machine Learning → Quantum Machine Learning

- The calculation of the model (step 2) can also be done on a quantum computer
- For this, a variational quantum approach is used

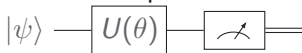


Variational Quantum Algorithms

- “Standard” quantum circuit:



- Variational quantum circuit:



- Operations in a variational quantum circuit are parameterized
 - The optimal parameter value(s) depend(s) on the specific application
- Goal: optimize the parameter value(s) for the application

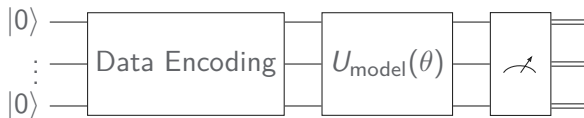
Steps

Input: Training data (already labelled data samples)

Task: Predict the labels for new data

1. Encode the classical data into a quantum state
2. Encode the model into a parameterized quantum circuit
3. Measure the circuit to determine the labels
4. Use (classical) optimization techniques to update the parameters of the quantum circuit

Quantum Circuit



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Angle Encoding

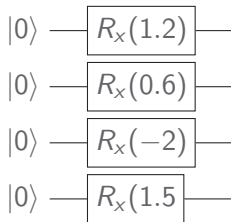
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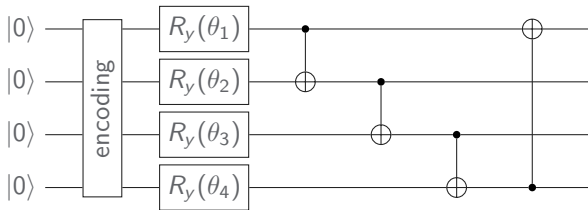
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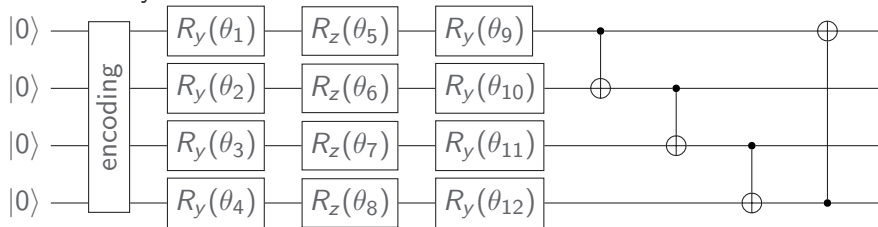
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- E.g., for binary classification we could take the **sign function** as classification function.

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- Variational quantum classifiers are **kernel methods** with measurement as **linear classifier**.
- Quantum advantage may be mainly in more diverse **data encoding**.

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- Other algorithms: Grover's algorithm, Shor's algorithm

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