Focused Tutorial on Quantum Computing

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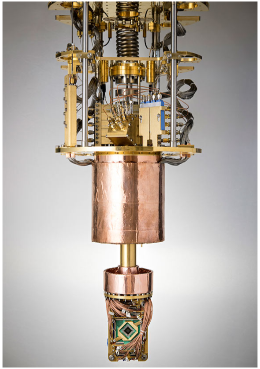
What is Quantum Computing?

- Exploiting quantum mechanical effects for computations



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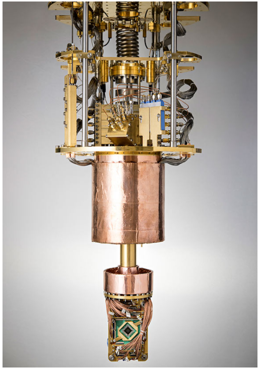

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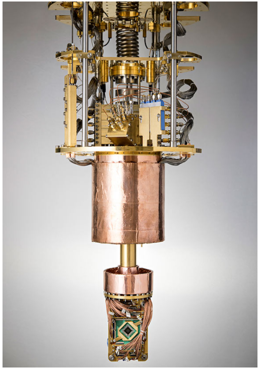
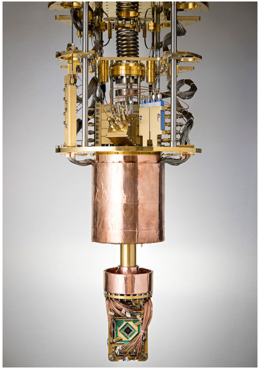


What is Quantum Computing?

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



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  - 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): Classication 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

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

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

where

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

Qubit States II

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

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

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Then we can write

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instead of

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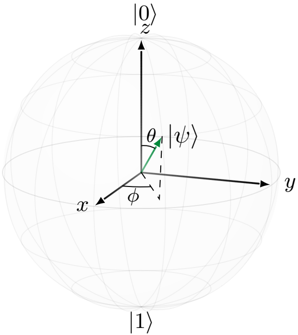
Bloch Sphere

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



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

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

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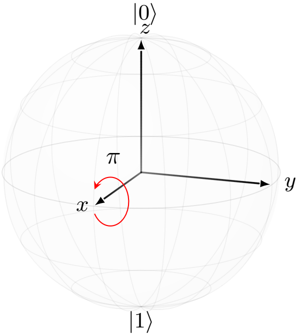
- We can represent operations on qubits in the quantum circuit model:

$$|\psi\rangle \; — \boxed{U} — \; |\psi'\rangle$$

Single Qubit Gates I

Pauli matrices:

- $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\quad -\boxed{X}-$



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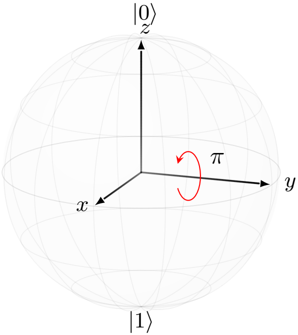

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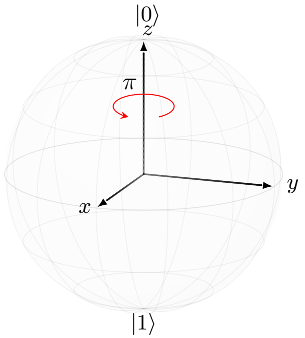
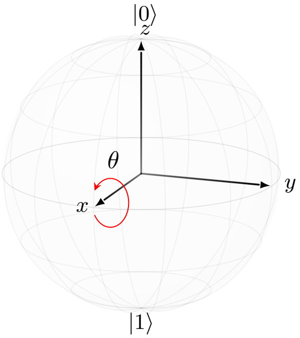


Arbitrary Rotations

R?(θ)-Gate: Rotation by θ around the X/Y/Z axis (?: X, Y, or Z)

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



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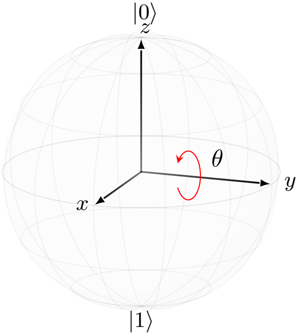

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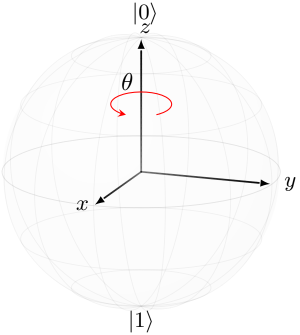
- $R_z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}$ $\boxed{R_z(\theta)}$



Measurement I

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

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

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

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$\rightarrow$ 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:

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

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

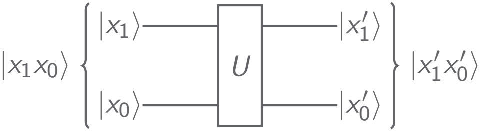
Two Qubit Register

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

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

Multi-Qubit Gates

We can also apply gates on multiple qubits:



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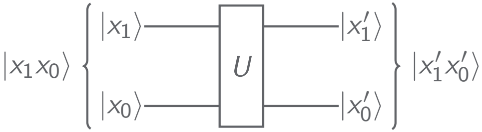


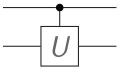
For instance, we can combine the existing single qubit gates using the tensor product:

$$X \otimes X =$$

Controlled Qubit Operations

- An operation on a qubit may depend on the state of another qubit $\rightarrow$ Any single-qubit gate can have a "controlled version"

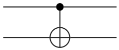
$$CU = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{10} \\ 0 & 0 & u_{01} & u_{11} \end{pmatrix}$$



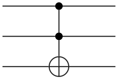
Controlled Qubit Operations

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

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



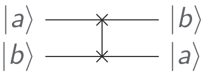
$$CCX = \begin{pmatrix} & & & 0 & 0 \\ & \mathbb{I}_6 & & \vdots & \vdots \\ & & & 0 & 0 \\ 0 & \cdots & 0 & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix}$$



The SWAP Operation

- The SWAP operation "swaps" the states of two qubits:

$$\mathrm{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



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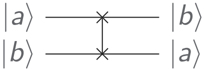
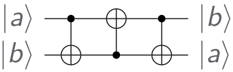
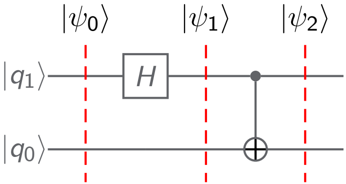


- It can be implemented with three CNOT gates:



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

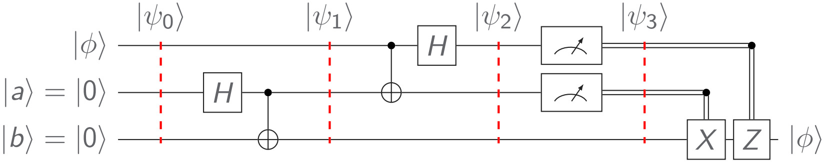
Qubits are *entangled* with each other iff the qubit state cannot be represented as a tensor product of single qubit states.

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

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

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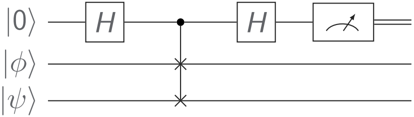
- Near-term quantum algorithms: Variational Quantum Algorithms (VQAs)

Swap Test I

Means to measure the distance d of two quantum states $|\phi\rangle$ and $|\psi\rangle$

$d = |\langle\psi|\phi\rangle|^2$ (angle^2 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 $P(\text{“Measure } |0\rangle\text{”}) = \frac{1}{2}$
  - If $|\psi\rangle$ and $|\phi\rangle$ are equal ($|\langle\psi|\phi\rangle|^2 = 1$), then $P(\text{“Measure } |0\rangle\text{”}) = 1$

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- Then $d = |\langle\psi|\phi\rangle|^2 = 2P(\text{“Measure } |0\rangle \text{”}) - 1$

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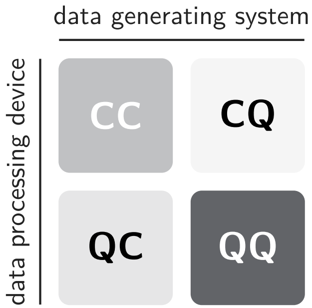
  - If $|\psi\rangle$ and $|\phi\rangle$ are equal ($|\langle\psi|\phi\rangle|^2 = 1$), then $P(\text{“Measure } |0\rangle\text{”}) = 1$
- Then $d = |\langle\psi|\phi\rangle|^2 = 2P(\text{“Measure } |0\rangle\text{”}) - 1$
- With multiple repetitions of the SWAP test, the distance d can be approximated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

Overview



C: Classical, Q: Quantum

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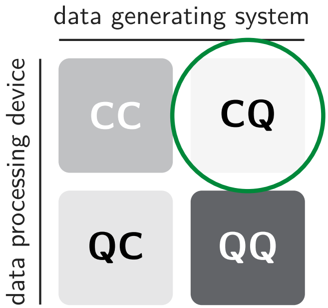

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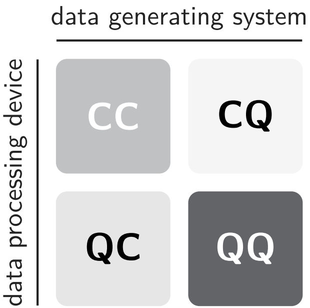
Overview – Classical Machine Learning



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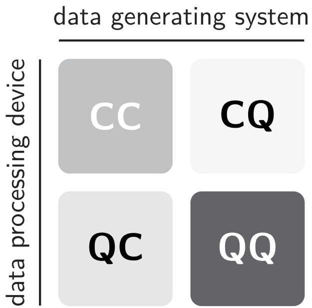

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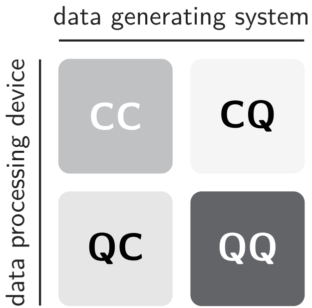

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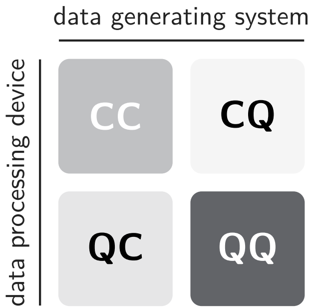

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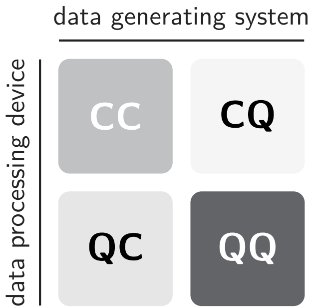

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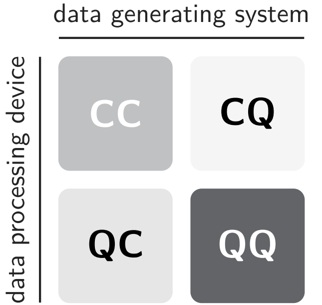

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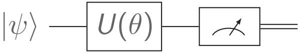
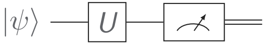
Classical Machine Learning → Quantum Machine Learning

- 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:



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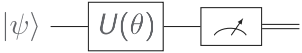

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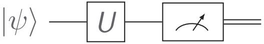

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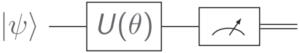

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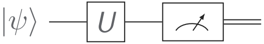

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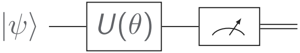

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$\rightarrow$ Goal: optimize the parameter value(s) for the application

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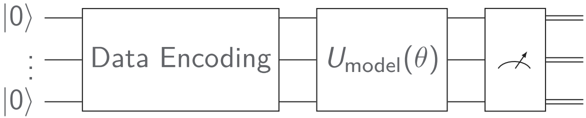
4. Use (classical) optimization techniques to update the parameters of the quantum circuit

Quantum Circuit



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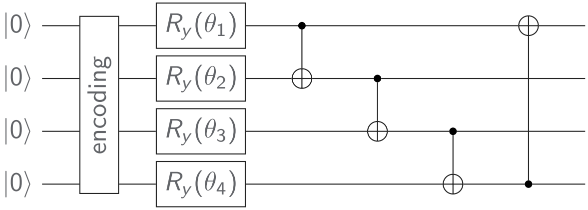

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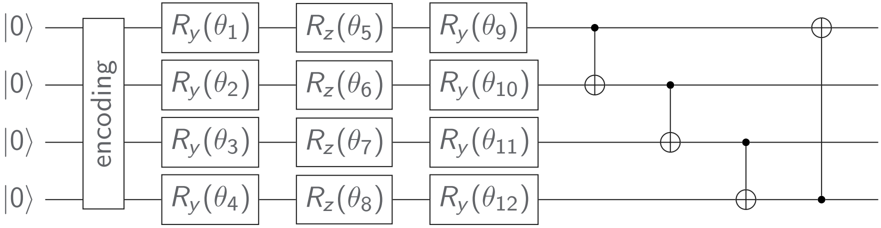

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- E.g., for binary classification we could take the **sign function** as classification function.

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- 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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