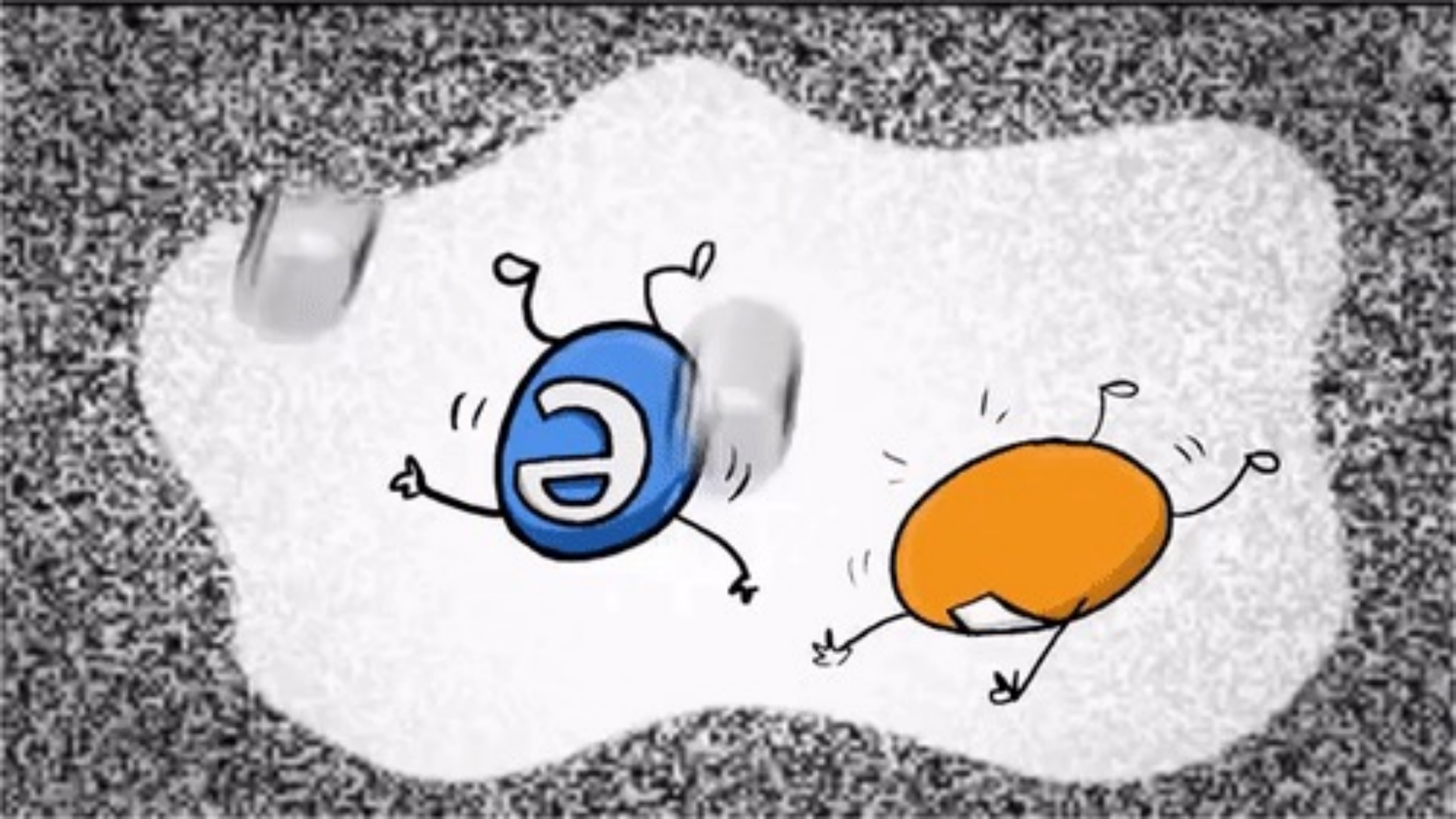
Quantum Machine Learning

Outline

- Introduction
- Quantum Machine Learning (QML) tasks
- Applications
- Data in QML
- Algorithm
- Challenges
- Quantum Resources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Introduction -- Quantum Mechanics (QM)

Mechanics: the study of the behavior of physical bodies when subjected to forces or displacements

Classical Mechanics: describing the motion of macroscopic objects.

Macroscopic: measurable or observable by naked eyes

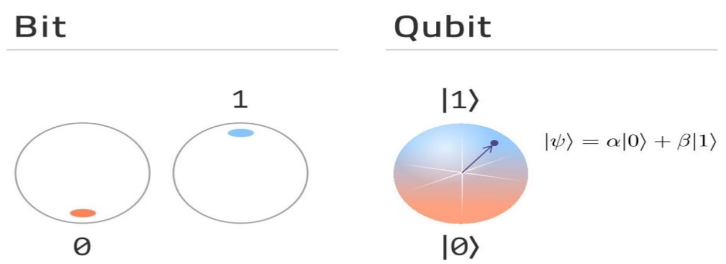
Quantum Mechanics: describing behavior of systems at atomic length scales and smaller .

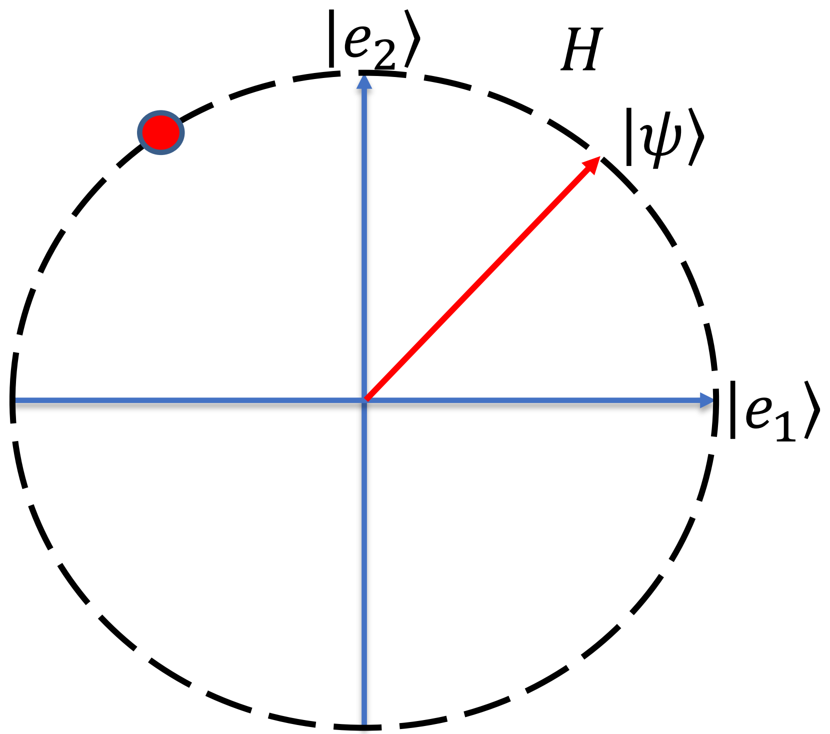
QM is established on four fundamental postulates

- State Space
- Evolution
- Measurement
- Composite System

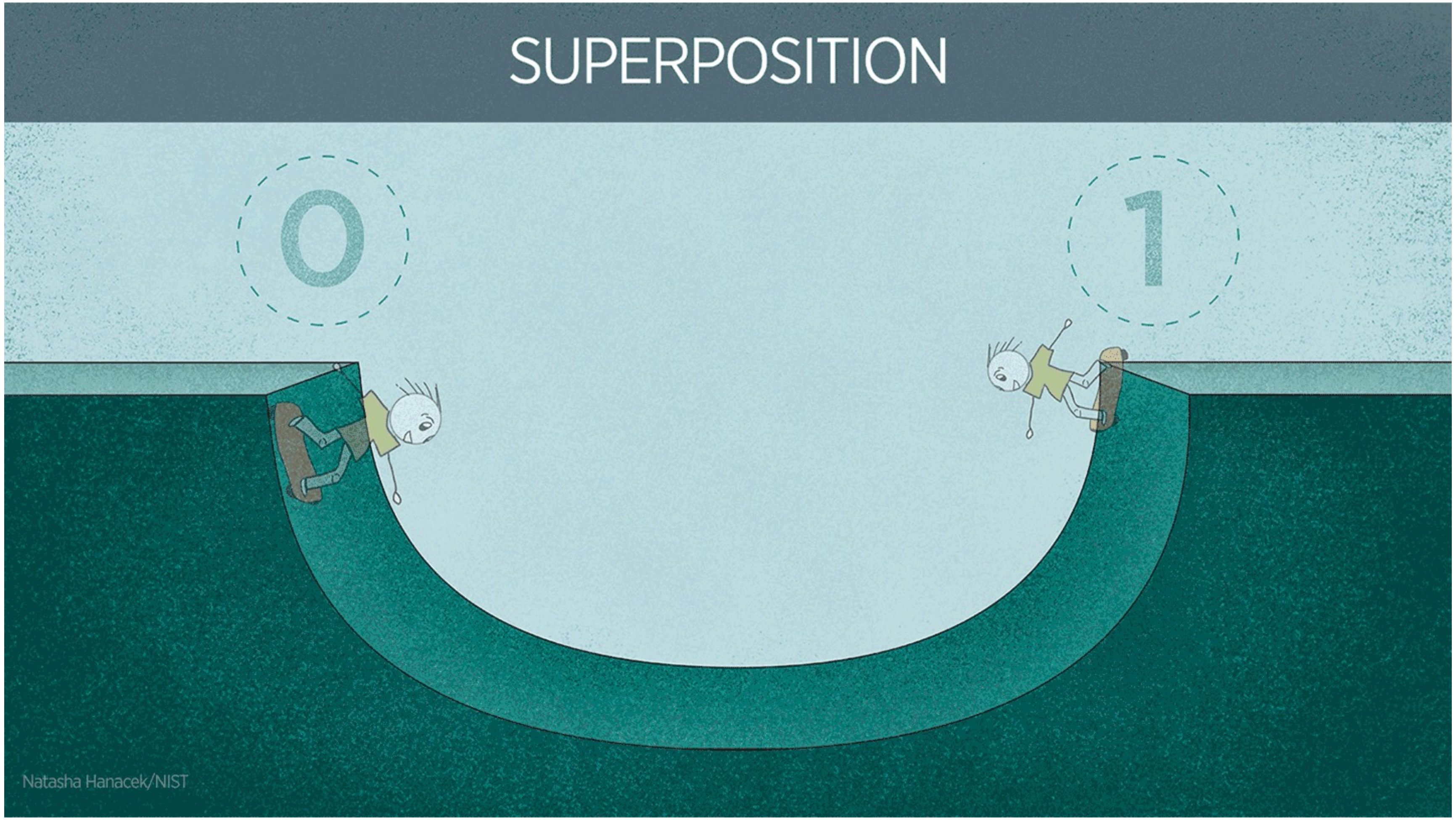
Introduction -- Quantum Mechanics (QM)

- Postulate 1: State Space
  - QM is defined on a Hilbert Space H
    - Infinite-dimensional Inner Product Vector Space
    - In practice, we consider finite-dimensional Complex Vector Space
  - A single quantum system is described by a pure state $|\psi\rangle$
    - **Basis State:** orthogonal states $\{|e_i\rangle\}$ that span H
    - **Superposition State:** other than basis states
      - $|\psi\rangle = \sum \alpha_i |e_i\rangle$, $\alpha_i \in C$, and $|e_i\rangle$ orthogonal unit vectors, $\sum |\psi_i|^2 = 1$
      - n qubit can be in superposition of 2^n states



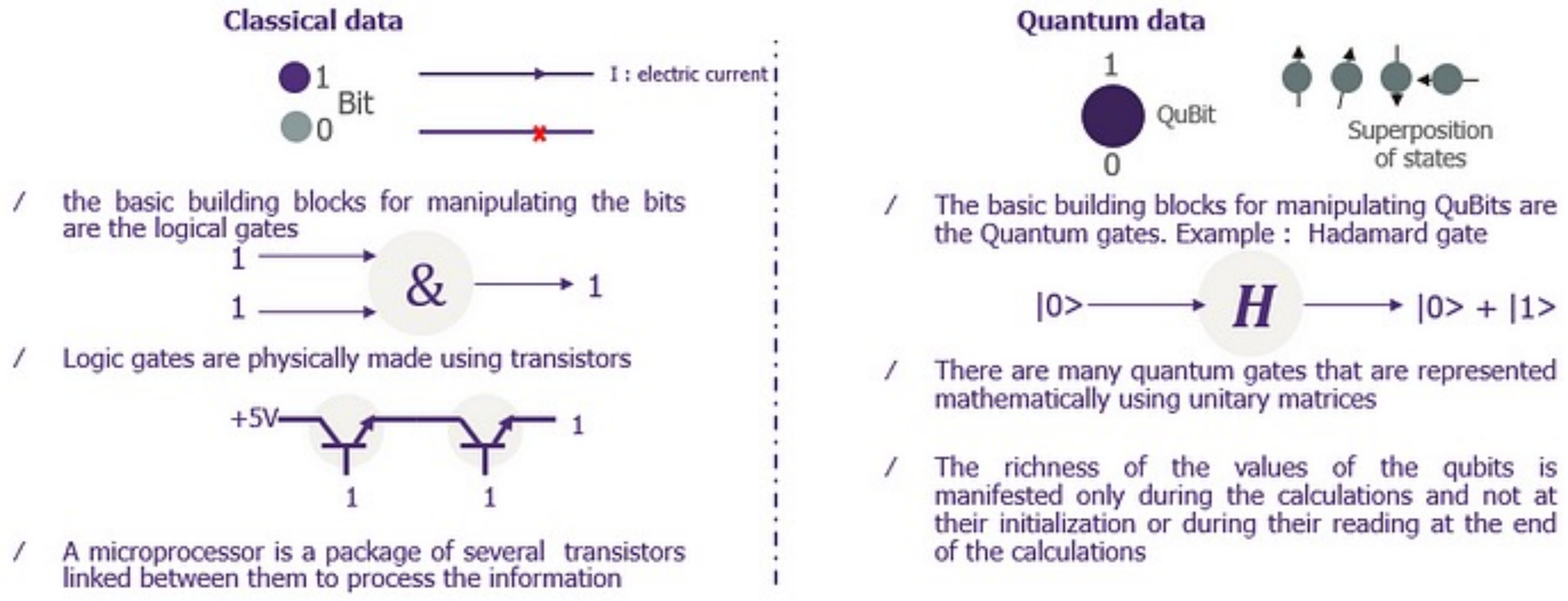


Introduction -- Quantum Mechanics (QM)



Introduction -- Quantum Mechanics (QM)

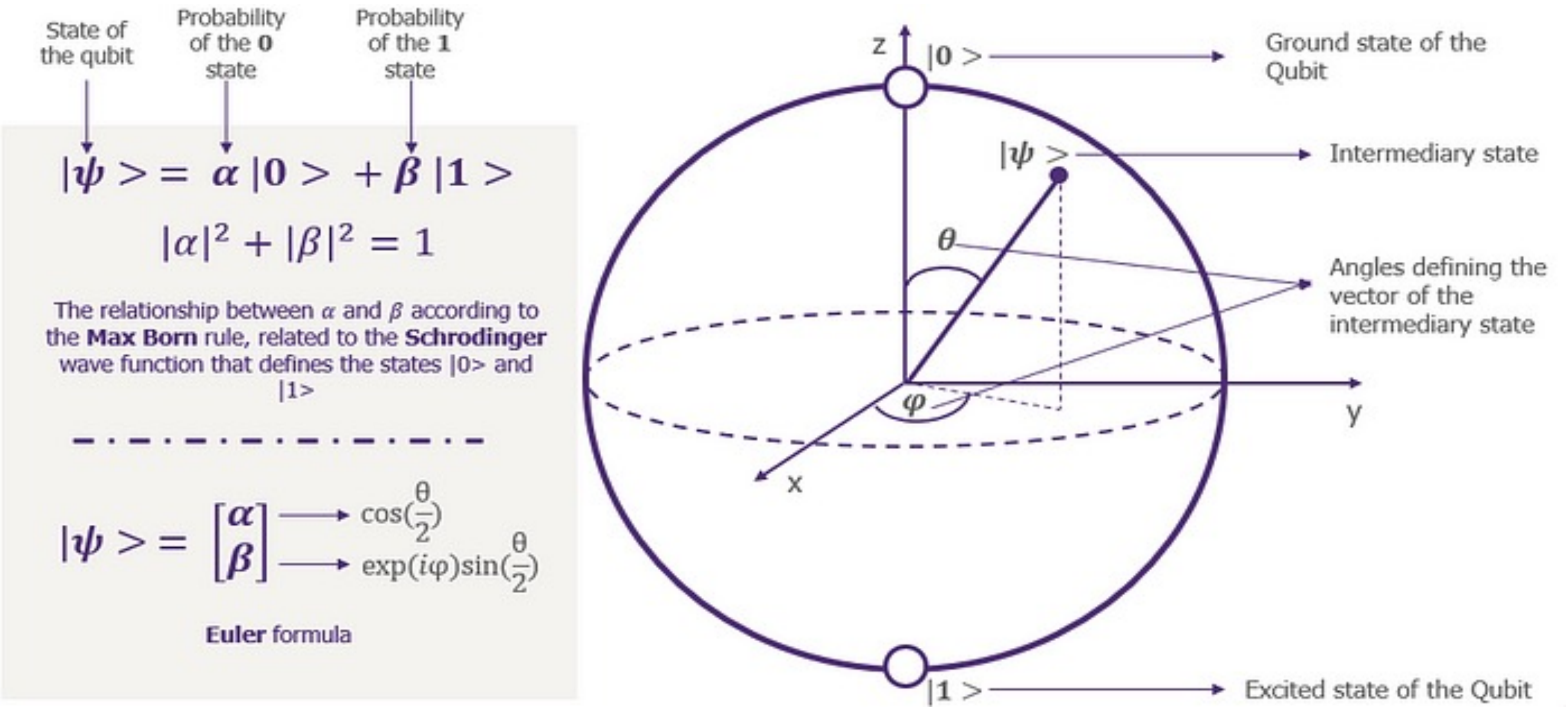
Qubits are the basic manipulation elements of information in quantum computers. They oppose the bits of classical computing. With them, ***we move from a deterministic world to a probabilistic world***



https://medium.com/meetech/highlighting-quantum-computing-for-machine-learning-1f1abd41cb59

Introduction -- Quantum Mechanics (QM)

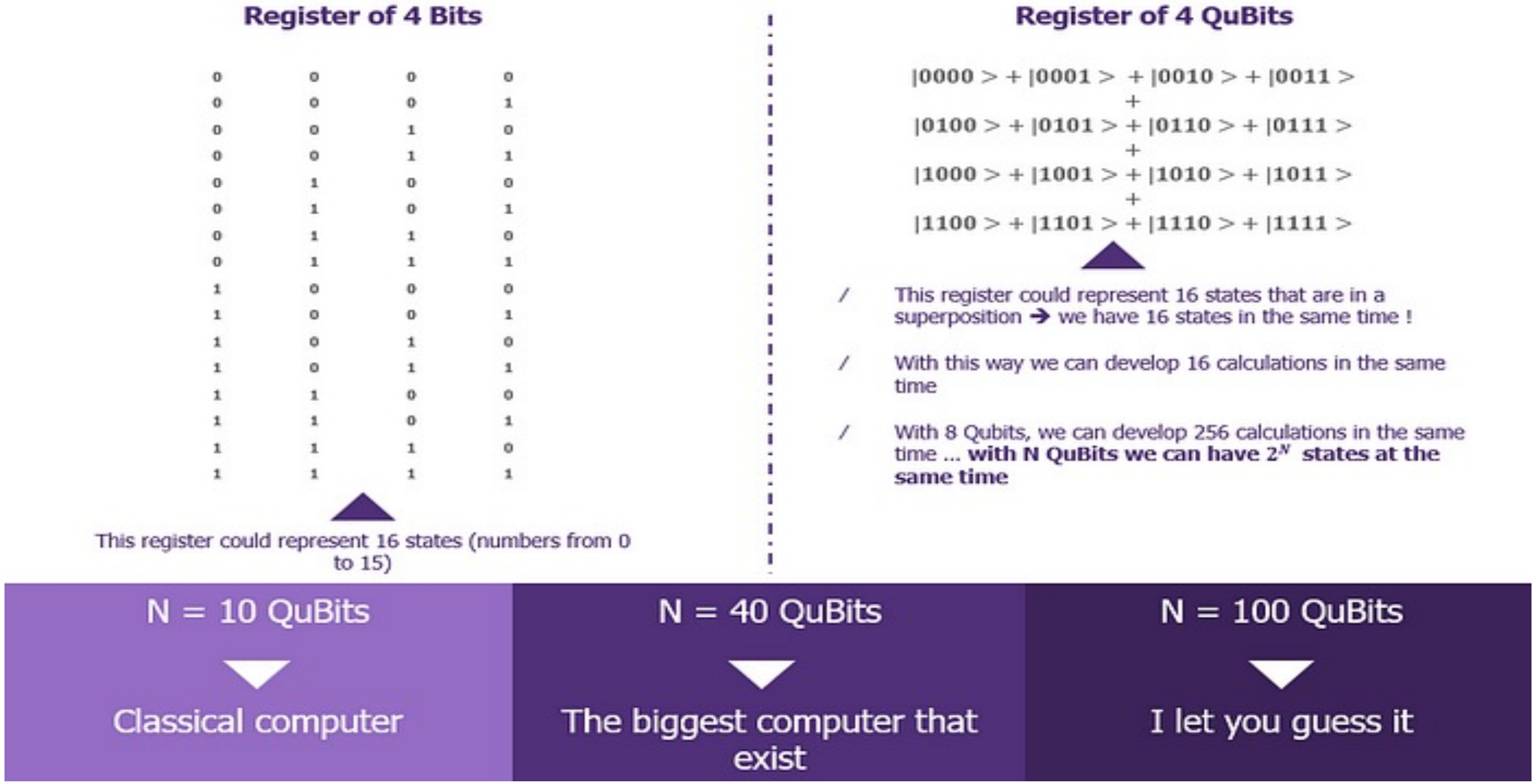
Bloch Sphere is the mathematical representation of a qubit. It represents the state of a qubit by a two-dimensional vector with a normal length of one.



Except for the initialization and measurement, it can be in superposition

https://medium.com/meetech/highlighting-quantum-computing-for-machine-learning-1f1abd41cb59

Introduction -- Quantum Mechanics (QM)



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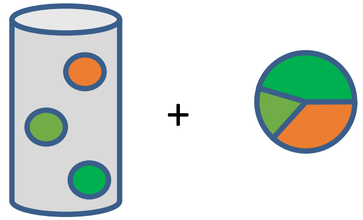
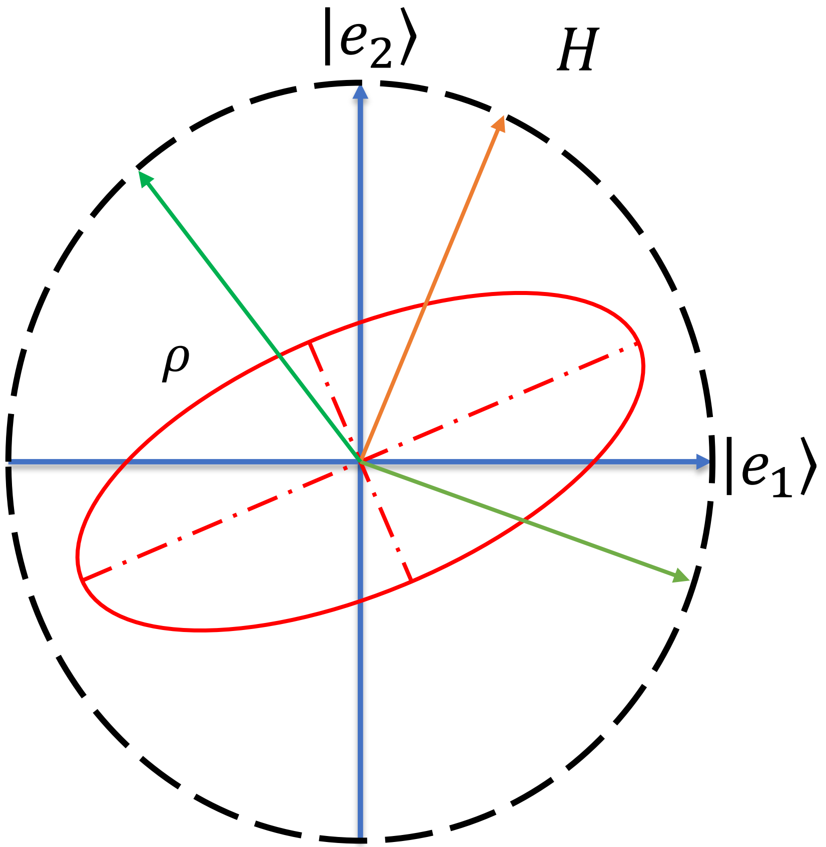
Introduction -- Quantum Mechanics (QM)

- Postulate 1: State Space
  - A probabilistic mixture of states (quantum mixture) is described by a mixed state ρ, also called a density matrix
    - $\rho = \sum \alpha_i |\psi_i\rangle\langle\psi_i|, \sum \alpha_i = 1$
    - ρ is a positive semi-definite matrix with unit trace
  - A density matrix uniquely defines a quantum probability distribution (Gleason's Theorem)
  - A density matrix represents a general single quantum state
    - A pure state $|\psi_i\rangle$ can be recast to a density matrix $\rho = |\psi_i\rangle\langle\psi_i|$

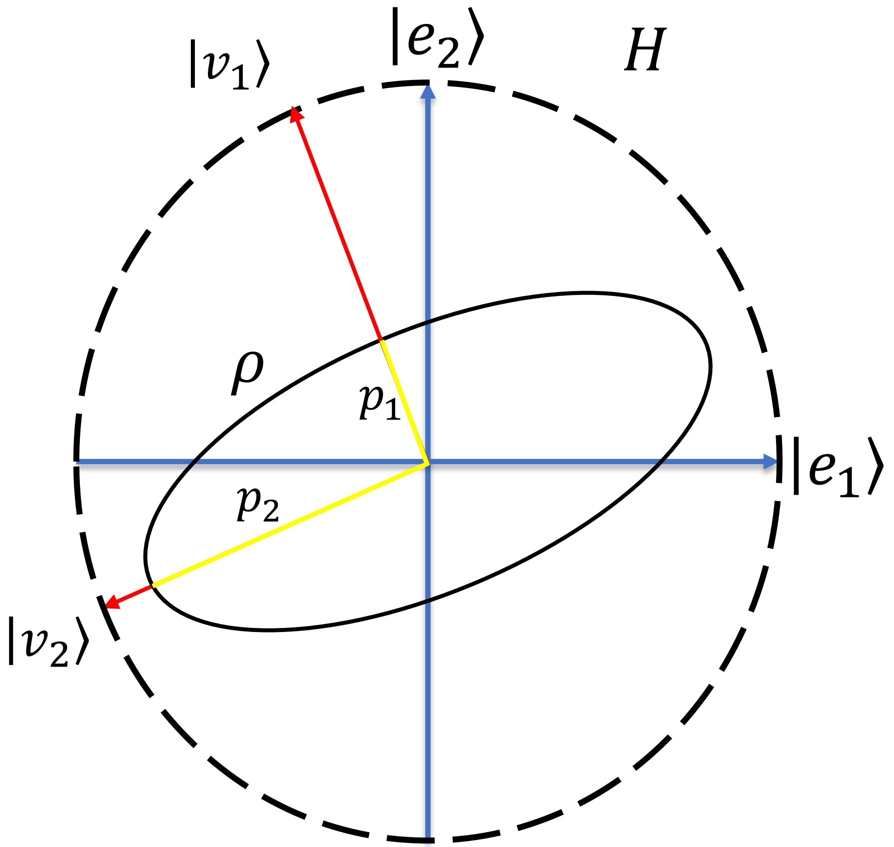




Introduction -- Quantum Mechanics (QM)

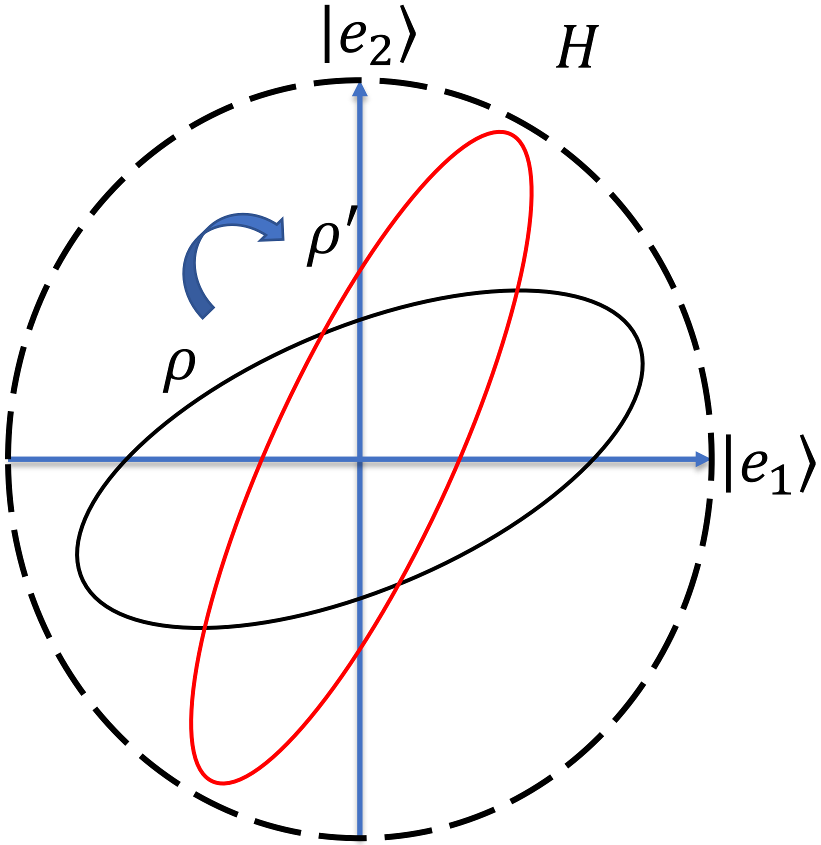
- Postulate 2: Measurement
  - The process of measuring the quantity of a system is Quantum Measurement
  - A quantum measurement is described by an observable $\hat{O}$
    - A set of orthogonal eigenstates $\{|\alpha_i\rangle \in H\}$
    - A set of eigenvalues $\{\alpha_i \in R\}$ (i.e. observed values)
  - The system collapses onto one eigenstate $|\alpha_i\rangle$, and the system takes the value α_i at probability

$$p_i = tr(\rho|\alpha_i\rangle\langle\alpha_i|)$$



Introduction -- Quantum Mechanics (QM)

- Postulate 3: Evolution
  - The evolution of a quantum system is described by a unitary transformation
$$\rho' = U\rho U^H$$
  - U is a unitary matrix, $U^H U = UU^H = I$
    - linear transformation on a quantum state preserving length of the state vector and the probability amplitudes of the basis states.
    - reversible and allow quantum states to be manipulated without losing information
  - For pure states $|v\rangle$ and $|v'\rangle$, $|v'\rangle = U|v\rangle$

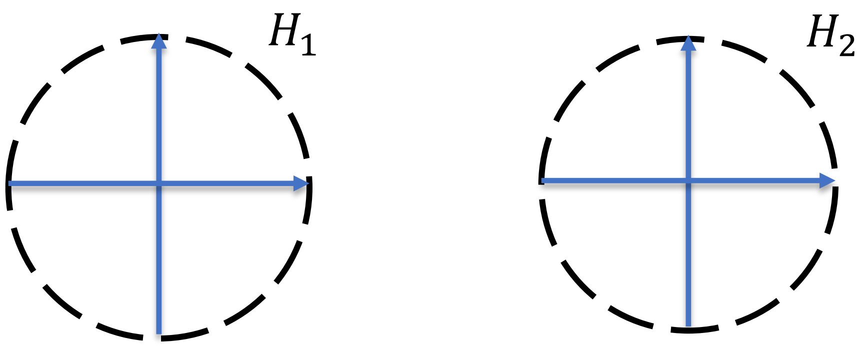


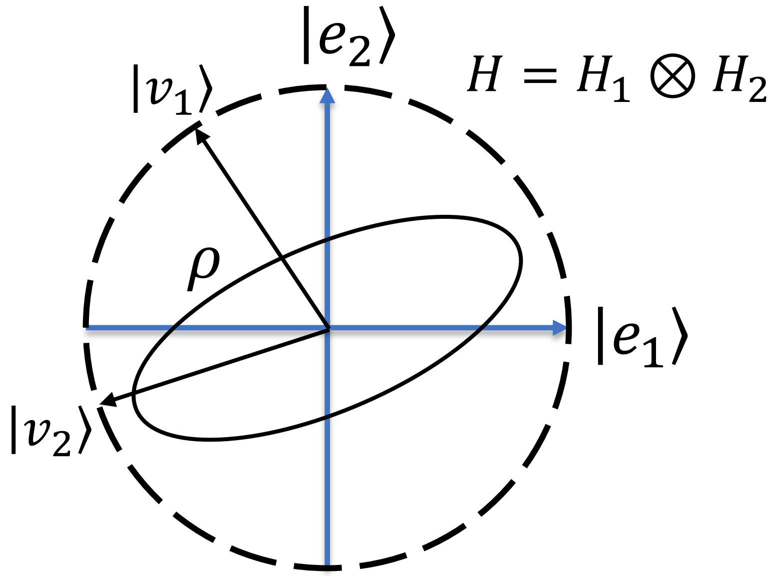
Introduction -- Quantum Mechanics (QM)

- Postulate 4: Composite System
  - Hilbert Space $H = H_1 \otimes H_2$
  - Basis states $|e_k\rangle = |e_{k_1}\rangle \otimes |e_{k_2}\rangle$

  - Entanglement: A state is separable if
    - Pure state $|\psi\rangle = |\psi^1\rangle \otimes |\psi^2\rangle$
    - Mixed state $\rho = \sum w_j \rho_j^1 \otimes \rho_j^2$

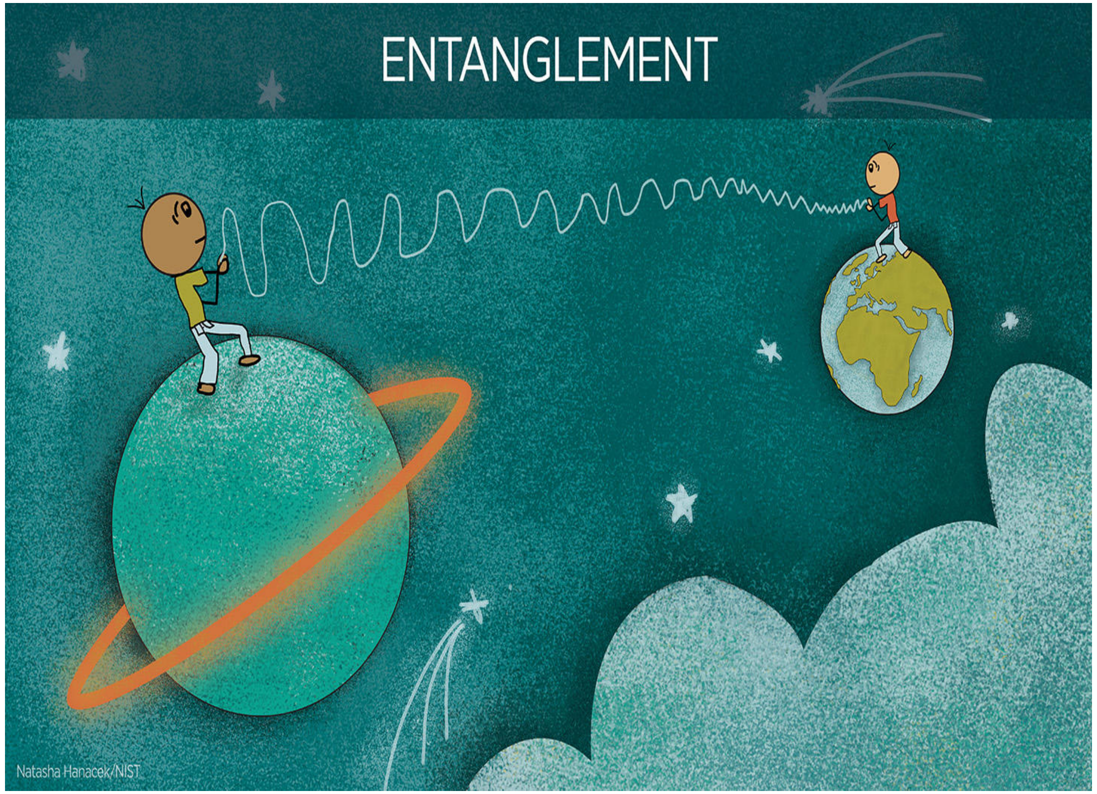
  - Otherwise the state is entangled
    - Measurement on one system leads to the change on the other



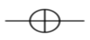
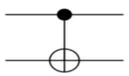
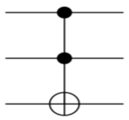


Introduction -- Quantum Mechanics (QM)

- Einstein believed that:
  - The outcome of a measurement on any physical system is determined prior.
  - the outcome cannot depend on any actions in space-like separated regions.
- Quantum mechanics predicts that:
  - Initially, the individual states of two particles are not identified.
  - The measurement outcome on particle A will not only determine its state, but also the state of particle B immediately!.
- two basis vectors $(|0\rangle_A, |1\rangle_A)$ of H_A, and $(|0\rangle_B, |1\rangle_B)$ of H_B, so entangled state: $\frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B)$



Introduction -- Quantum Mechanics (QM)

Operator	Gate(s)		Matrix
Pauli-X (X)	$\boxed{X}$		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	$\boxed{Y}$		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	$\boxed{Z}$		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	$\boxed{H}$		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	$\boxed{S}$		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	$\boxed{T}$		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0 \end{bmatrix}$

Pauli equivalent to NOT gates and rotate the state of qubit around X,Y,Z-axis on Bloch Sphere

Hadmard transform the basis states |0⟩ and |1⟩ into superposition:

|0⟩ → (|0⟩ + |1⟩) / √2

|1⟩ → (|0⟩ - |1⟩) / √2

CNOT operates on two qubits, a control qubit and a target qubit, and it applies a NOT gate to the target qubit if the control qubit is in the state |1⟩:

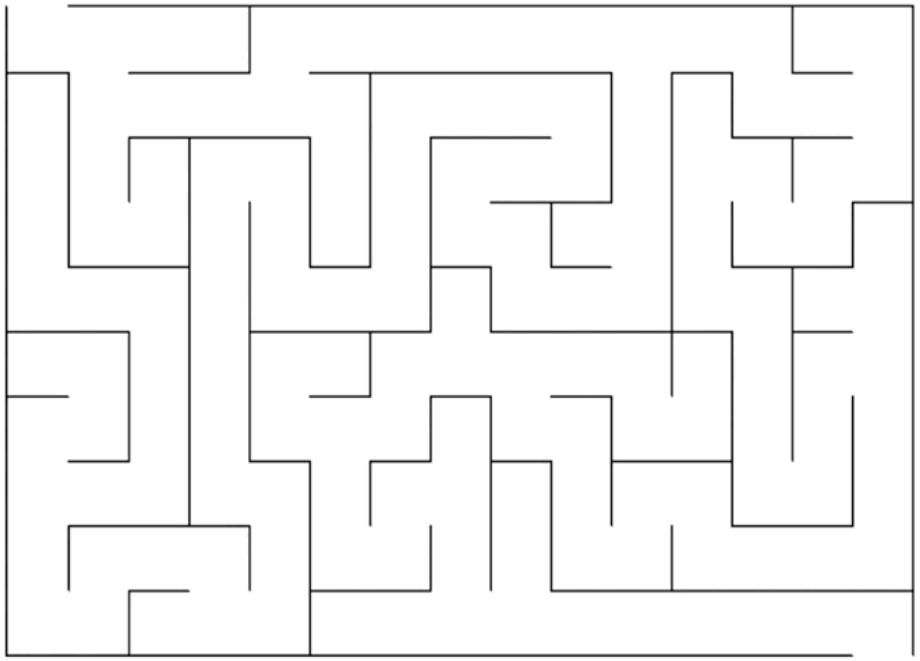
|00⟩ → |00⟩

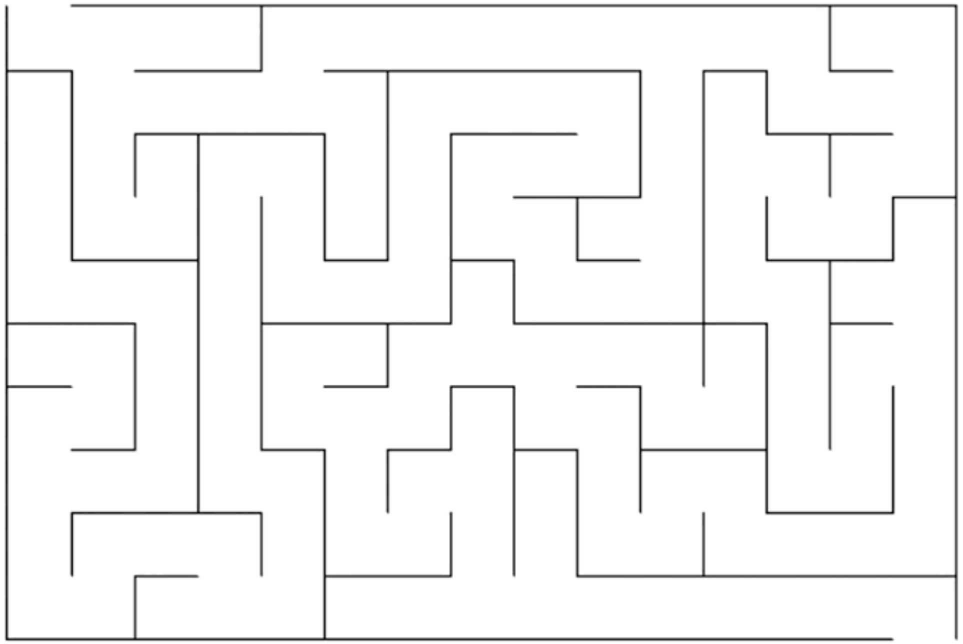
|01⟩ → |01⟩

|10⟩ → |11⟩

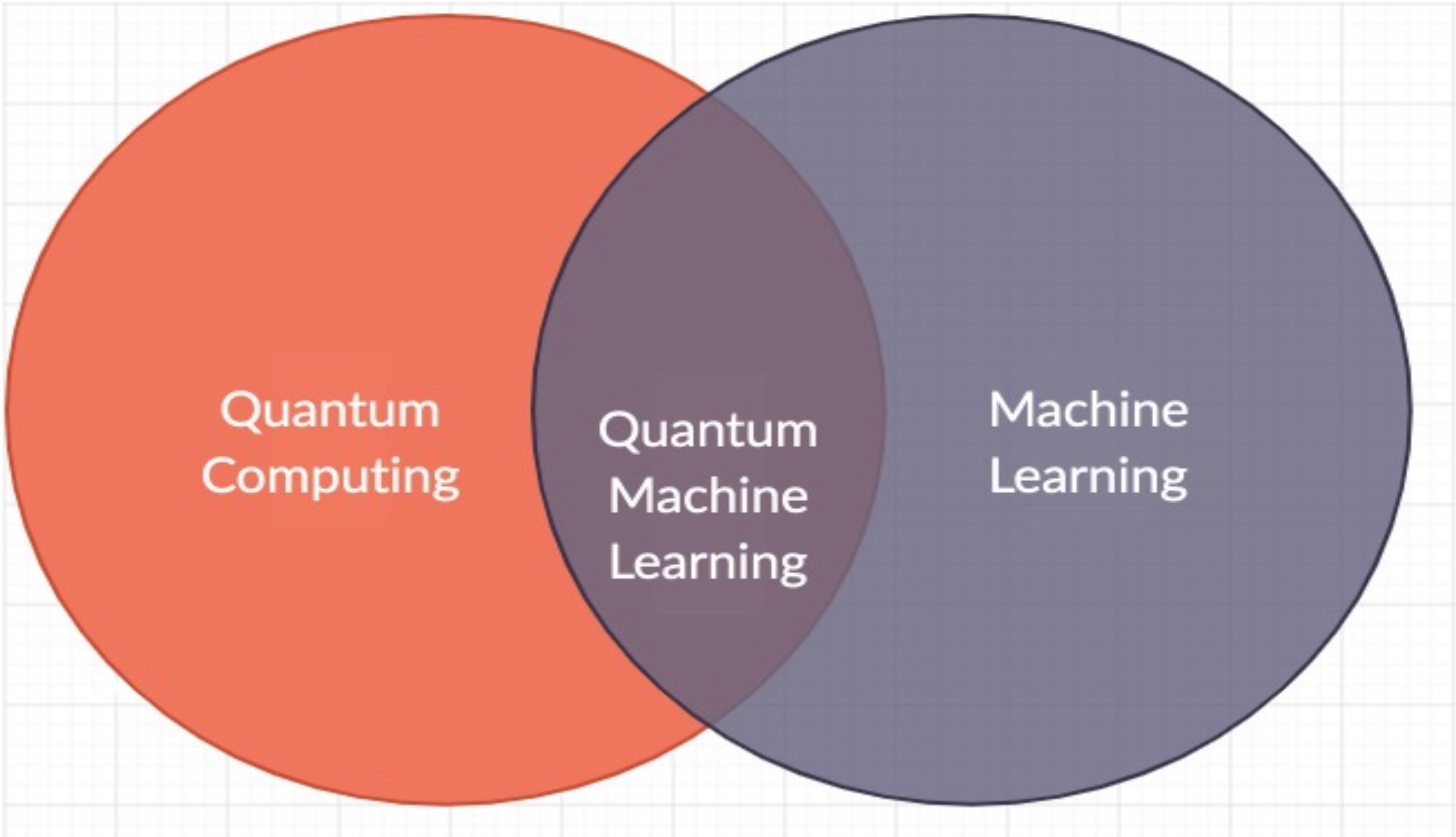
|11⟩ → |10⟩

Introduction -- Quantum Mechanics (QM)

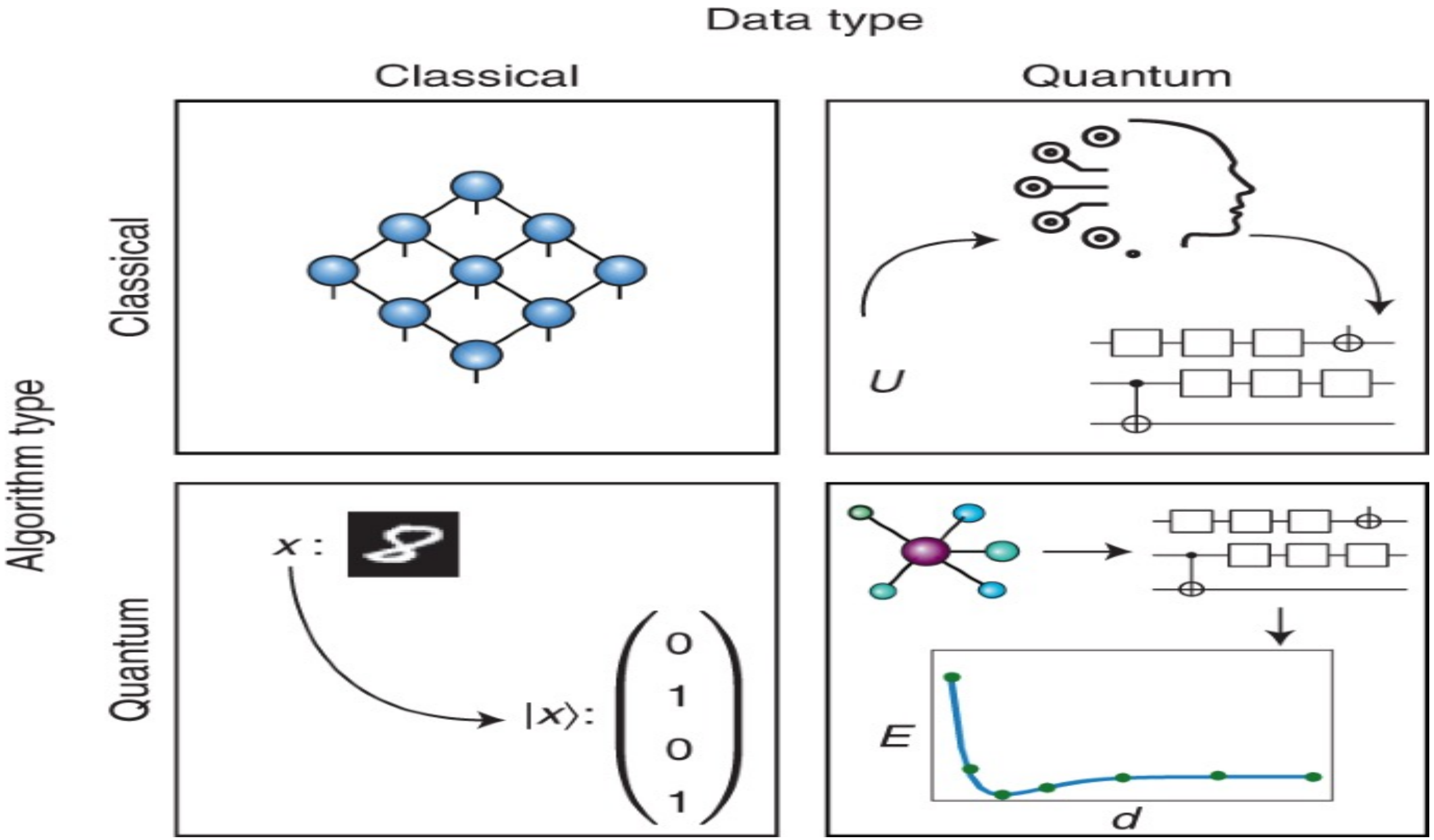




Quantum Machine Learning (QML)



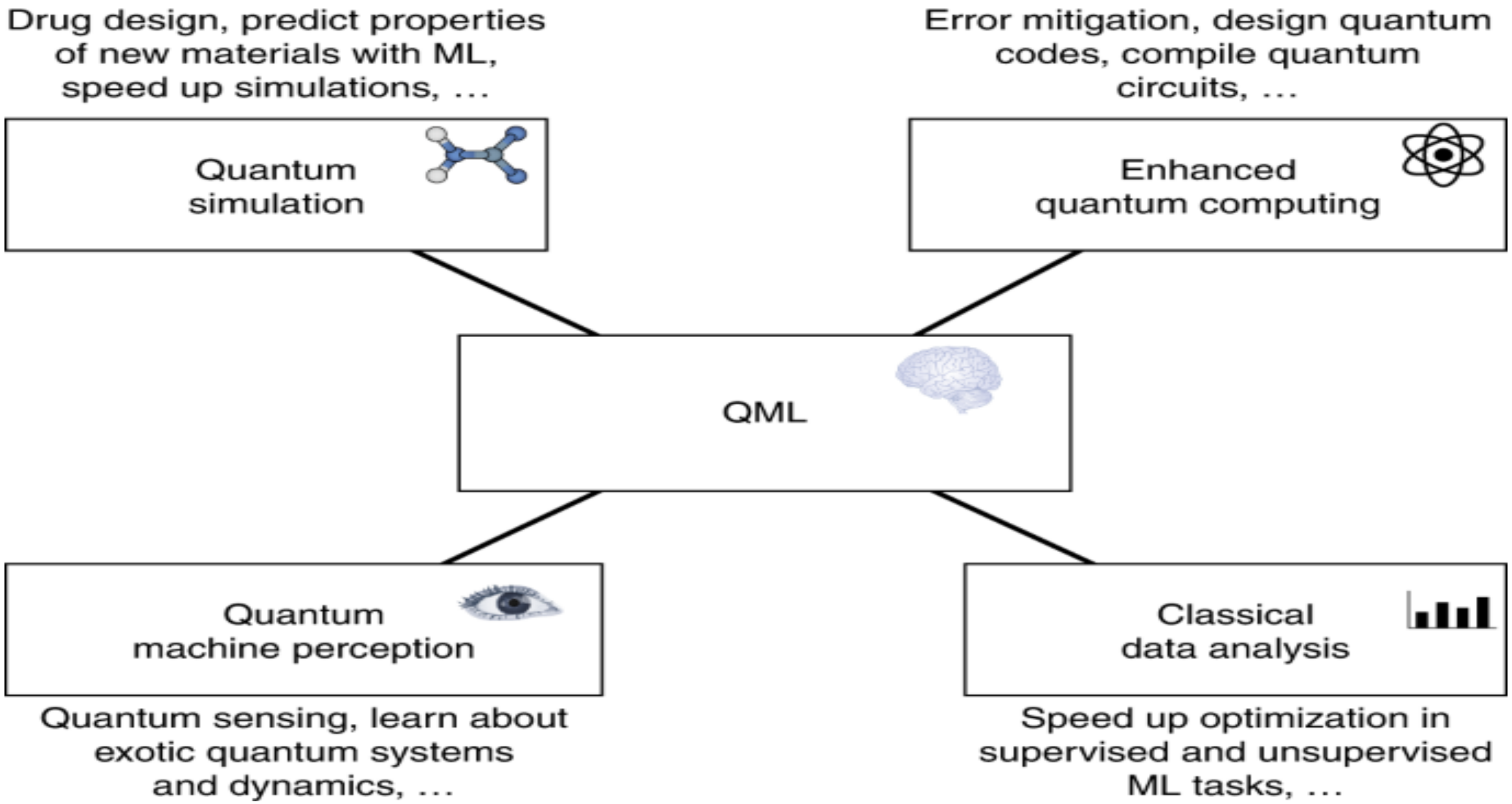
Quantum Machine Learning (QML) tasks



Quantum machine learning is usually considered for four main tasks. These include tasks where the data is either classical or quantum, and where the algorithm is either classical or quantum. Top left: tensor networks are quantum-inspired classical methods that can analyze classical data. Top right: unitary time-evolution data *U* from a quantum system can be classically compiled into a quantum circuit. Bottom left: handwritten digits can be mapped to quantum states for classification on a quantum computer. Bottom right: molecular ground state data can be classified directly on a quantum computer. The figure shows ground state energy E dependence on the distance d between the atoms.

Cerezo, M., et al. "Challenges and opportunities in quantum machine learning." Nature Computational Science 2.9 (2022): 567-576.

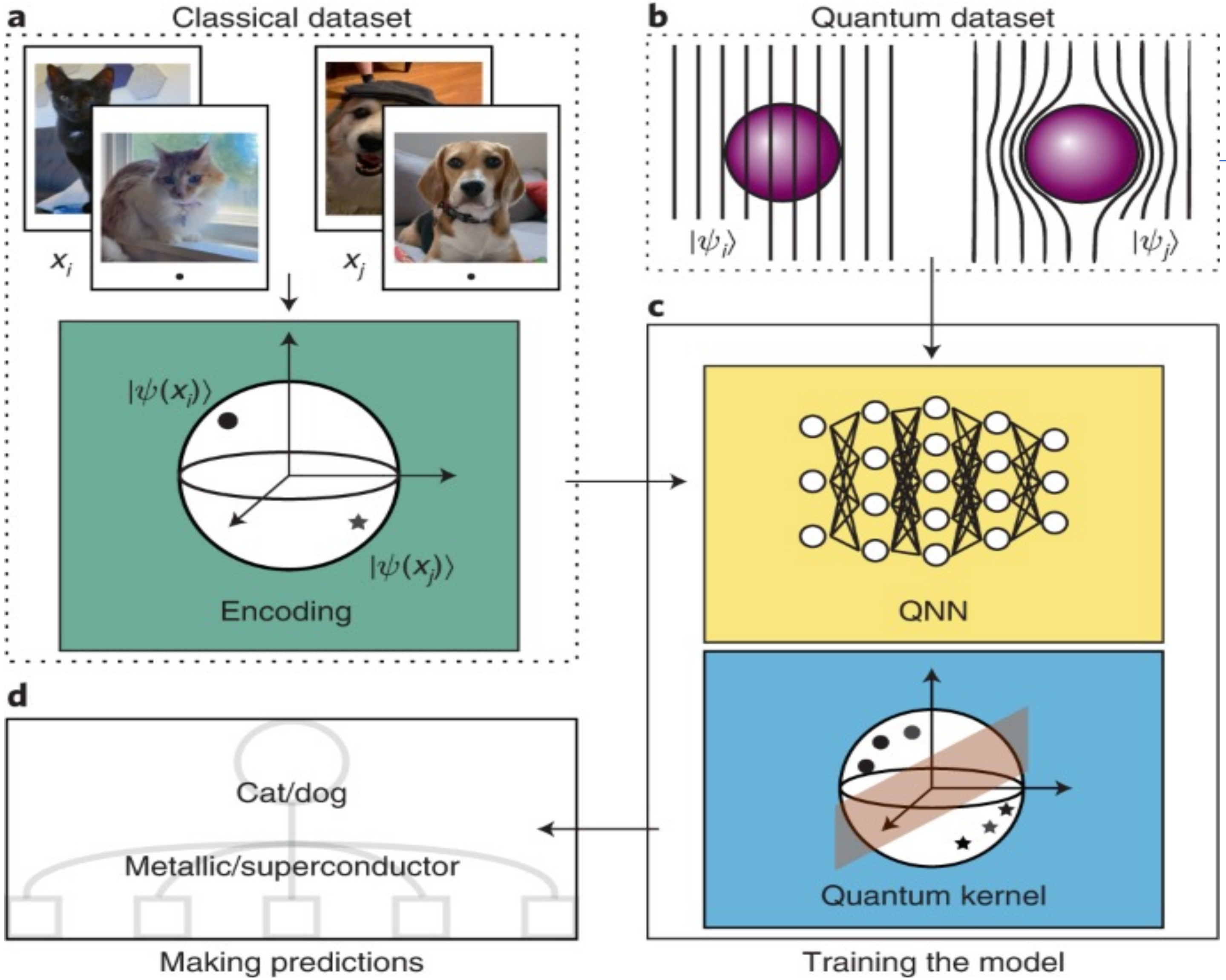
QML Applications



QML has been envisioned to bring a computational advantage in many applications. QML can enhance quantum simulation for chemistry (e.g., molecular ground states, equilibrium states and time evolution) and materials science (e.g., quantum phase recognition and generative design with a target property in mind). QML can enhance quantum computing by learning quantum error correction codes and syndrome decoders, performing quantum control, learning to mitigate errors, and compiling and optimizing quantum circuits. QML can enhance sensing and metrology and extract hidden parameters from quantum systems. Finally, QML may speed up classical data analysis, including clustering and classification. Some applications produces data that is inherently quantum mechanical.

Cerezo, M., et al. "Challenges and opportunities in quantum machine learning." Nature Computational Science 2.9 (2022): 567-576.

Data in QML



set of quantum states $\{|\boldsymbol{\psi_j}\rangle\}$ or unitaries *{Uj}*

a) The classical data x, i.e., images of cats and images of dogs, is encoded into a Hilbert space via some map $\boldsymbol{x} \rightarrow |\boldsymbol{\psi}(\boldsymbol{x})\rangle$. Ideally, data from different classes (here represented by dots and stars) is mapped to different regions of the Hilbert space.
b) Quantum data $\boldsymbol{\psi}(\boldsymbol{x})$ can be directly analyzed on a quantum device. Here the dataset is composed of states representing metallic or superconducting systems.
c) The dataset is used to train a QML model. Two common paradigms in QML are quantum neural networks and quantum kernels, both of which allow for the classification of either classical or quantum data. In Kernel methods one fits a decision hyperplane that separates the classes.
d) Once the model is trained, it can be used to make predictions.

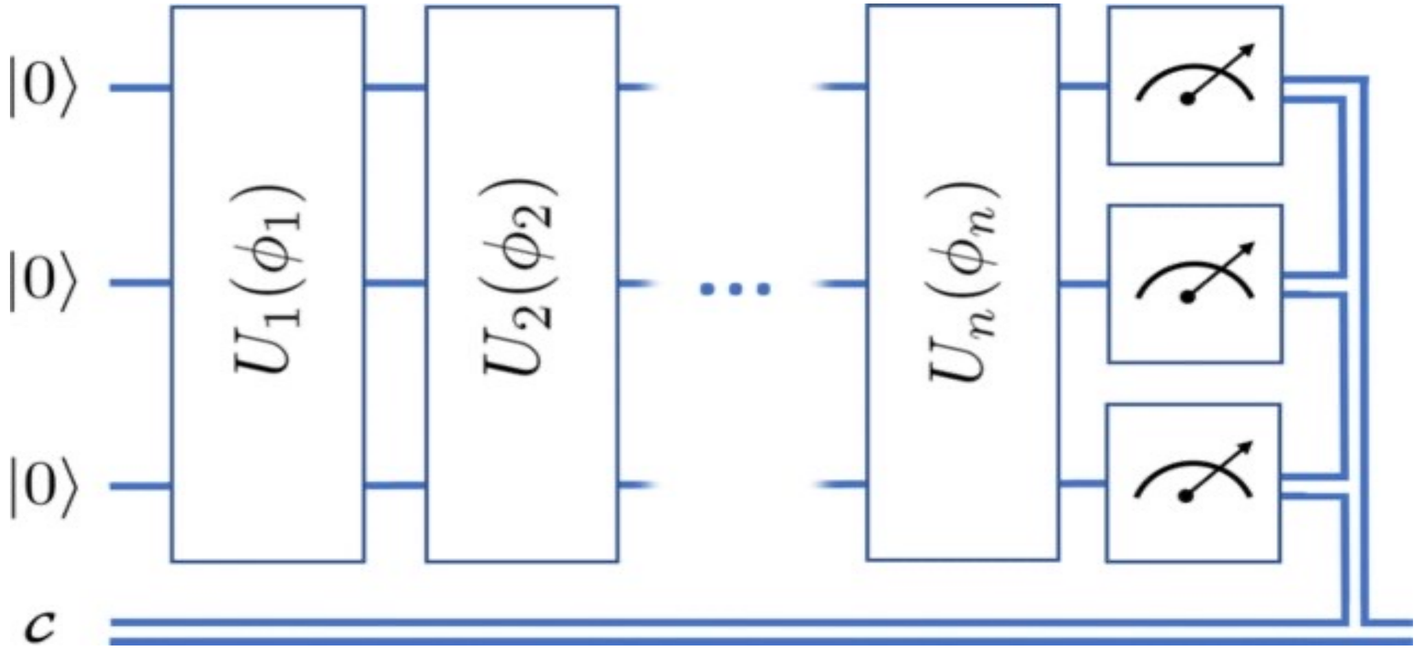
Cerezo, M., et al. "Challenges and opportunities in quantum machine learning." Nature Computational Science 2.9 (2022): 567-576.

QML Algorithms

- **Quantum-inspired algorithms [1-6]**
  - simulated quantum annealing to optimize classical cost functions
  - Do not require a quantum computer
- **Quantum data processing algorithms**
  - Exploiting the quantum properties of data for CML
- **Quantum-enhanced classical machine learning algorithms**
  - CML uses quantum features for improvement
- **Variational quantum algorithms [8,9]**
  - Use variational methods to optimize a cost function on a quantum computer
  - VQA (QNN) solve ML problem on a quantum computer using PQC.
- **Quantum clustering algorithms [7]**
  - cluster data using quantum methods
  - Qk-means uses the phase estimation algorithm to cluster data points into k groups.
- **Quantum kernel [10,11]**
- **Quantum Reinforcement Learning**

Quantum Neural Networks (QNN)

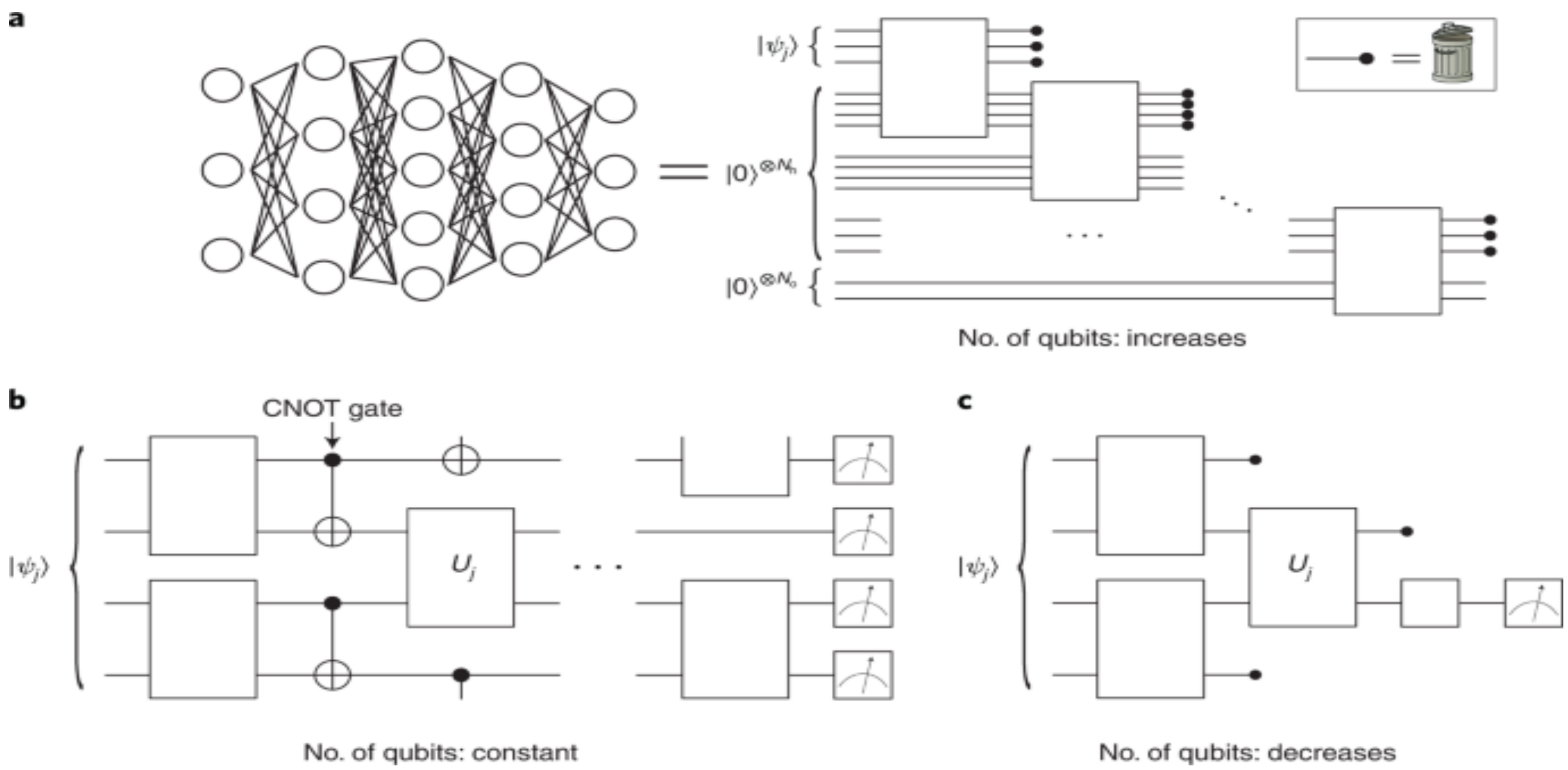
sequence of unitary gates acting on the quantum data states



General parameterized quantum circuit, with arbitrary unitaries U, input state |0⟩, and classical register c, where φ = [φ1,φ2,...,φn] are the parameters of the circuit. Though the unitaries do not necessarily act on all qubits, we have arranged them here in "blocks," similar to the general architectures of VQE where a block of operations may be repeated many times in a circuit, with different parameters. In the case of VQE, a block might be a series of single-qubit rotations or a set of entangling gates (such as CNOT), or block might be a phase unitary encoding the cost function or a mixing unitary for searching the solution space.

Wilson, Max, et al. "Optimizing quantum heuristics with meta-learning." Quantum Machine Intelligence 3 (2021): 1-14.

Examples of QNN architectures



a) Dissipative QNN -- classical feed-forward network, nodes are qubits, and lines connecting them are unitary operations. Term dissipative arises from the fact that qubits in a layer are discarded after the information forward-propagates to the (new) qubits in the next layer.
b) Standard QNN -- quantum data states are sent through a quantum circuit, at the end of which some or all of the qubits are measured. Here, no qubits are discarded or added as one goes deeper into the QNN.
c) Convolutional QNN -- each layer qubits are measured to reduce the dimension of the data while preserving its relevant features.

Beer, Kerstin, et al. "Training deep quantum neural networks." Nature communications 11.1 (2020): 808.

Hybrid Quantum Neural Networks (QNN)

- input vector $x \in R^{n \times 1}$ to $|\psi\rangle$, trainable parameter W
- define parameterized unitary operation U_x , U_w acting on $|\psi\rangle$ in order $U_x\, U_w\, |\psi\rangle$ or $U_w\, U_x\, |\psi\rangle$
- Expectation of observable Z on all qubits computed
- For quantum state $|\phi\rangle = U_W U_X |\psi\rangle$,

$$\mathrm{E} = f(Re(\langle \phi | Z^{\otimes n} | \phi \rangle))$$

- Simulating quantum measurmeents and estimating the expectation value of Hamiltonians on quantum system

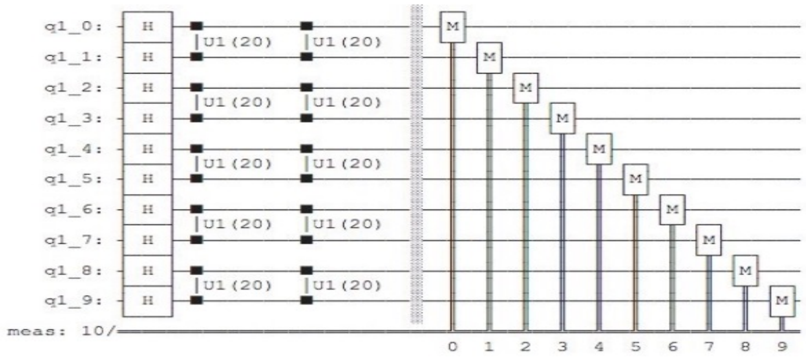


Fig. 2: The schematic diagram of the quantum circuit, in which all parameters are fixed to 20. In reality, as the reader will explore in algorithm 1, these parameters are more complex and varying over time. Moreover, the original gates are controlled R_y gates, which are optimized to U_1 by Qiskit.

Algorithm 1: QuantumLayer(): Algorithm for operation of quantum layer

Require QUBITS = 8; input_parameters[8]

quantumRegister = qiskit.QuantumRegister(QUBITS)
quantumCircuit = qiskit.QuantumCircuit(QUBITS)
classicalCircuit = qiskit.ClassicalCircuit(QUBITS)
for $q_i \in quantumRegister$ *and* $c_i \in classicalRegister$ **do**
  -Apply hadamard gate $\mathcal{H}$ to q_i
  -Apply controlled-Y gate with input_parameters[i] between q_i and q_{i+1}
  -Apply controlled-Y gate with input_parameters[i] between q_i and q_{i-1}
  -**Measurement:** Map q_i to c_i
Compute Z expectation on the returned measurements
Send the output to the next layer in the neural network

Algorithm 2: Algorithm to construct hybrid classical-quantum neural network **ARCH1**

inputLayer = tensorflow.keras.layers.Input(120)
layer1 = tensorflow.keras.layers.Dense(8) (inputLayer)
layer2 = **QuantumLayer** (layer1)
layer3 = tensorflow.keras.layers.Dense(10) (layer2)
outputLayer = tensorflow.keras.layers.Dense(23) (layer3)

Source	Arch.	Loss	Acc.
ARCH1	120 - 8 - 8_q - 10 - 23	0.0240	0.9956
ARCH2	120 - 10 - 8 - 8_q - 8_q - 23	0.0874	0.9825
[23]	decision trees	-	0.9292
[24]	41 - 21 - 21 - 5	-	0.8023
[25]	RNN and variations	-	0.9924
[26]	LSTM	-	0.9899
[27]	41 - 100 - 100 - 100 - 100 - 5 - 5	-	0.999
[28]	LSTM	-	0.9912
[29]	CNN	-	0.9984
[30]	hidden layers with 17 nodes	-	0.9850

Laxminarayana, Nikhil, et al. "Quantum-assisted activation for supervised learning in healthcare-based intrusion detection systems." IEEE Transactions on Artificial Intelligence (2022).

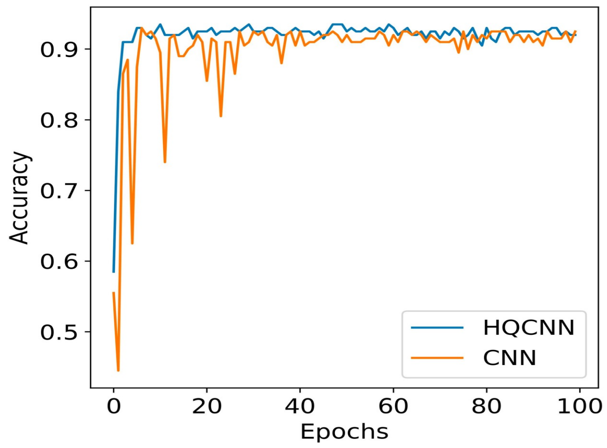
Hybrid Quantum Neural Networks (QNN)

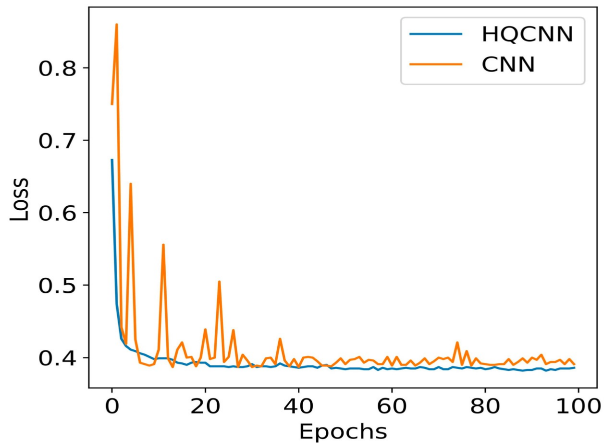
- quantum encoding for each convolution,
- $U_E: x \in R \rightarrow |\phi(x)\rangle = \bigotimes_{i=0}^{n-1} (\cos\alpha_i |0\rangle + \sin\alpha_i |1\rangle)$

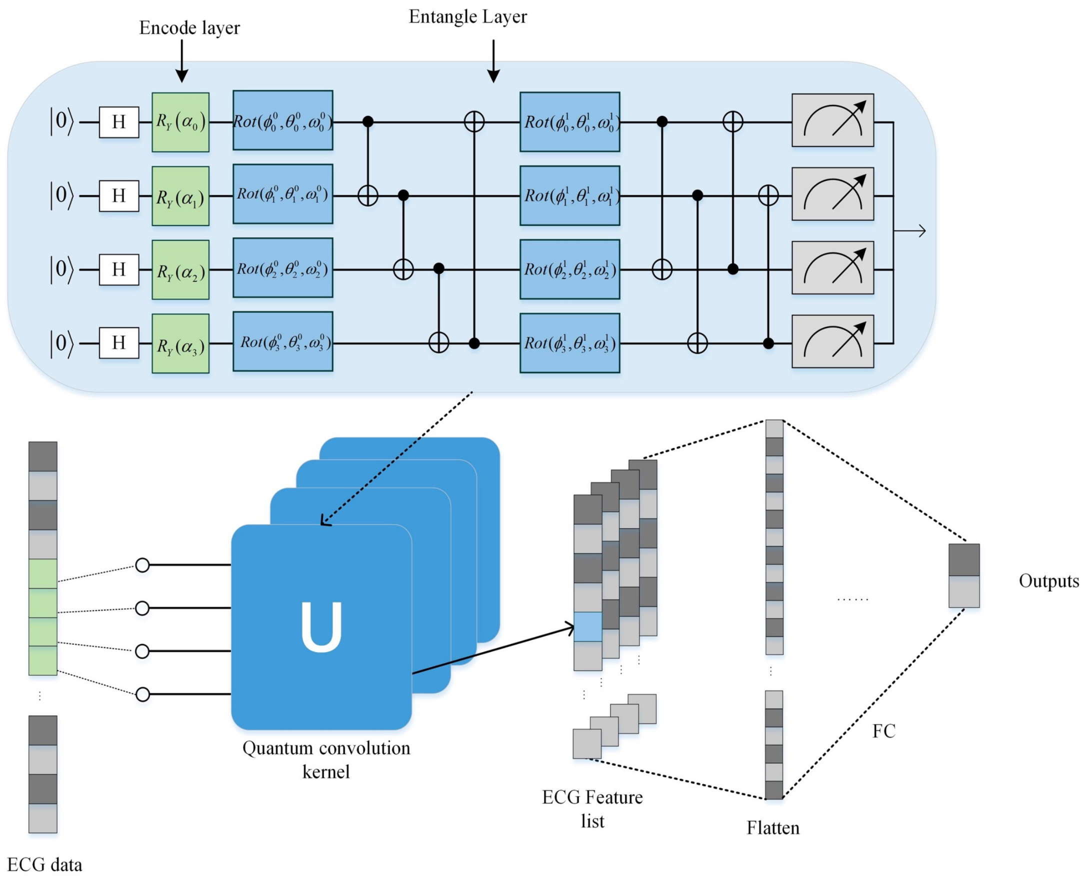
Here, $\alpha_i = \pi \cdot x_i \in [0, \pi)$, coding matrix $U_E = \bigotimes_{i=0}^{n-1} U_i$ and

$$U_i = R_Y(2\alpha_i) = \begin{pmatrix} \cos\alpha_i & -\sin\alpha_i \\ \sin\alpha_i & \cos\alpha_i \end{pmatrix}$$

- entanglement circuit in the quantum convolution kernel uses the Rot gate.
- By adjusting the appropriate parameters, Rot gate can rotate state $|0\rangle$ to any positions on the Bloch Sphere.
- Correlation measurement expectation $\langle\varphi|U^\dagger Z^{\otimes n} U|\varphi\rangle$ is used as the output of the quantum circuit, because it express the entanglement information of the quantum circuit.

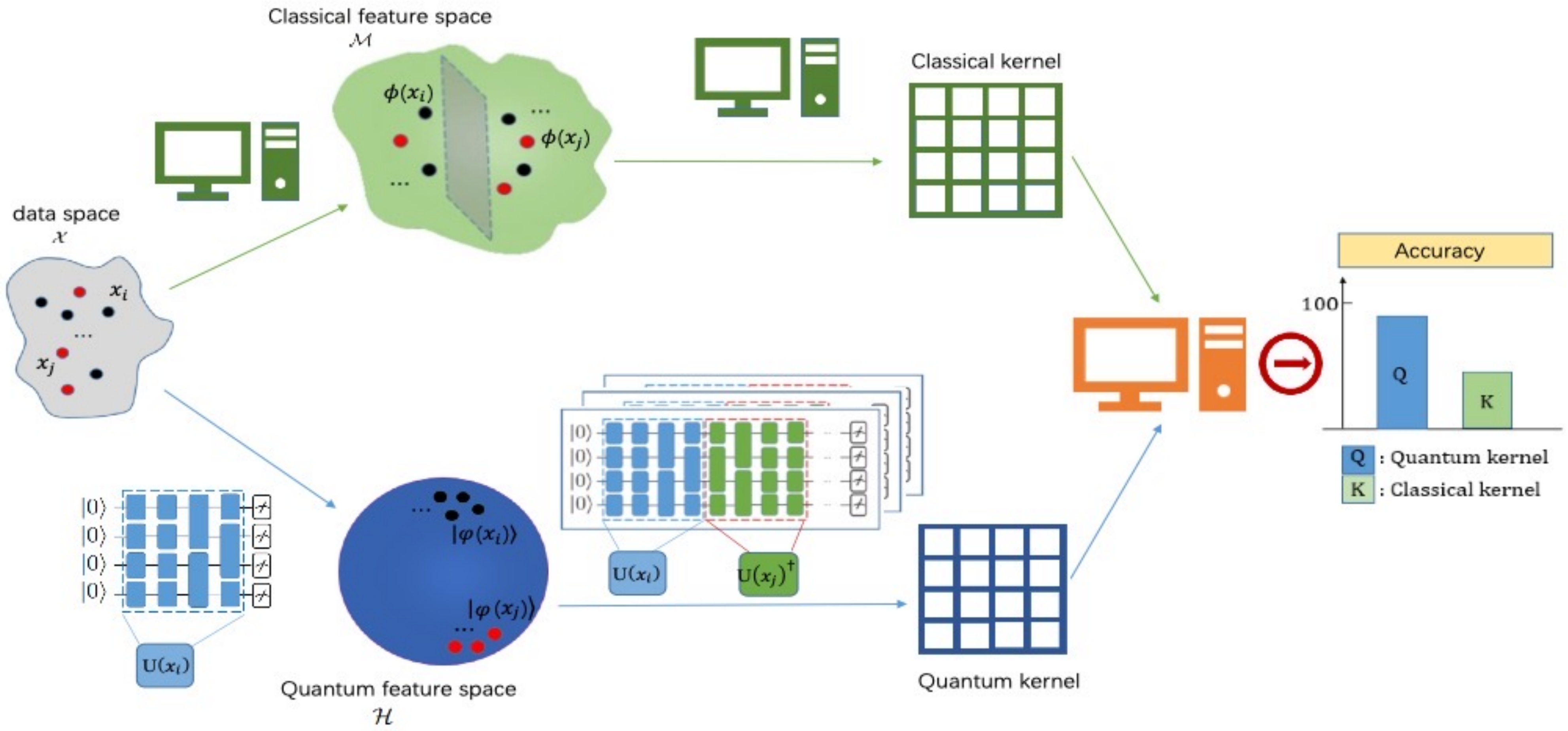






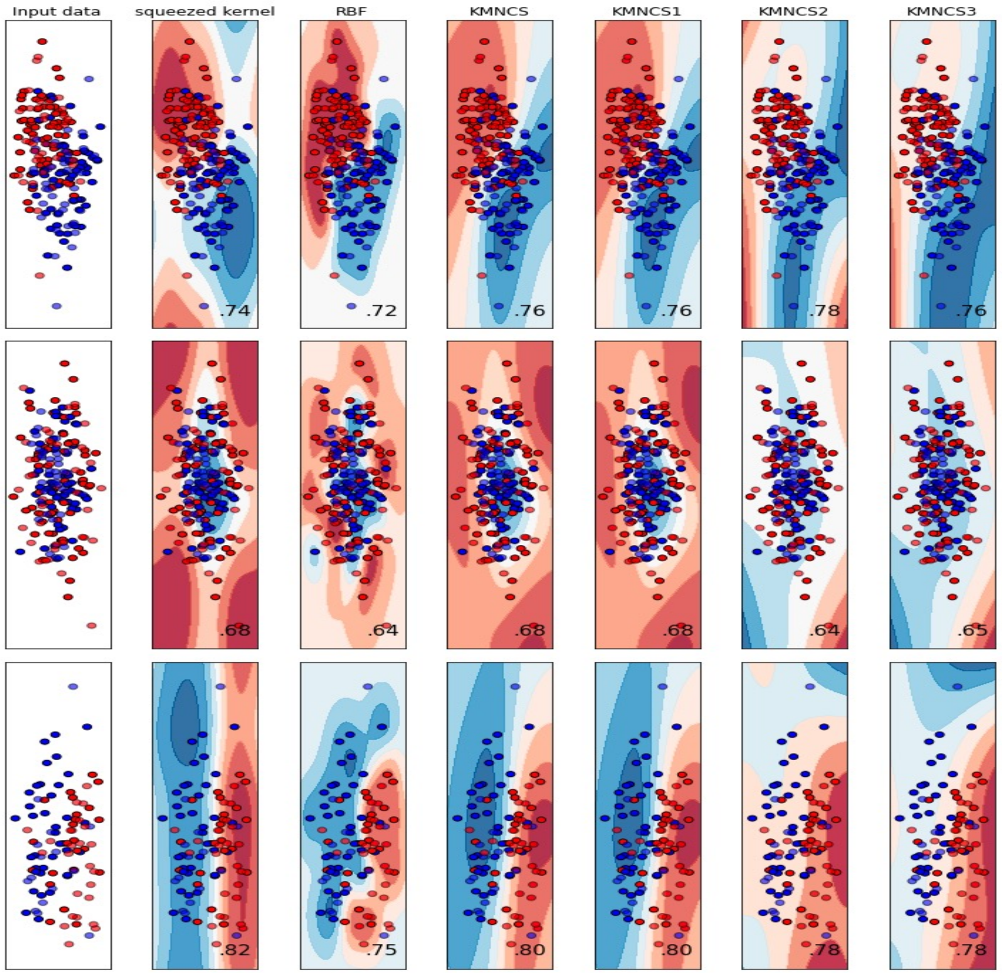
The convolutional layer is replaced by parameterized quantum circuits, and the linear layer is composed of classical fully connected neural networks.

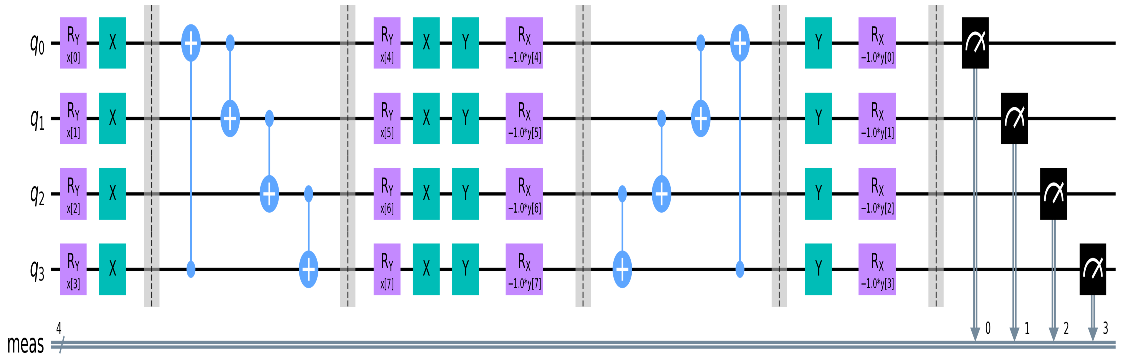
Quantum Kernels



"Towards understanding the power of quantum kernels in the NISQ era." Quantum 5 (2021): 531.

Quantum Kernels



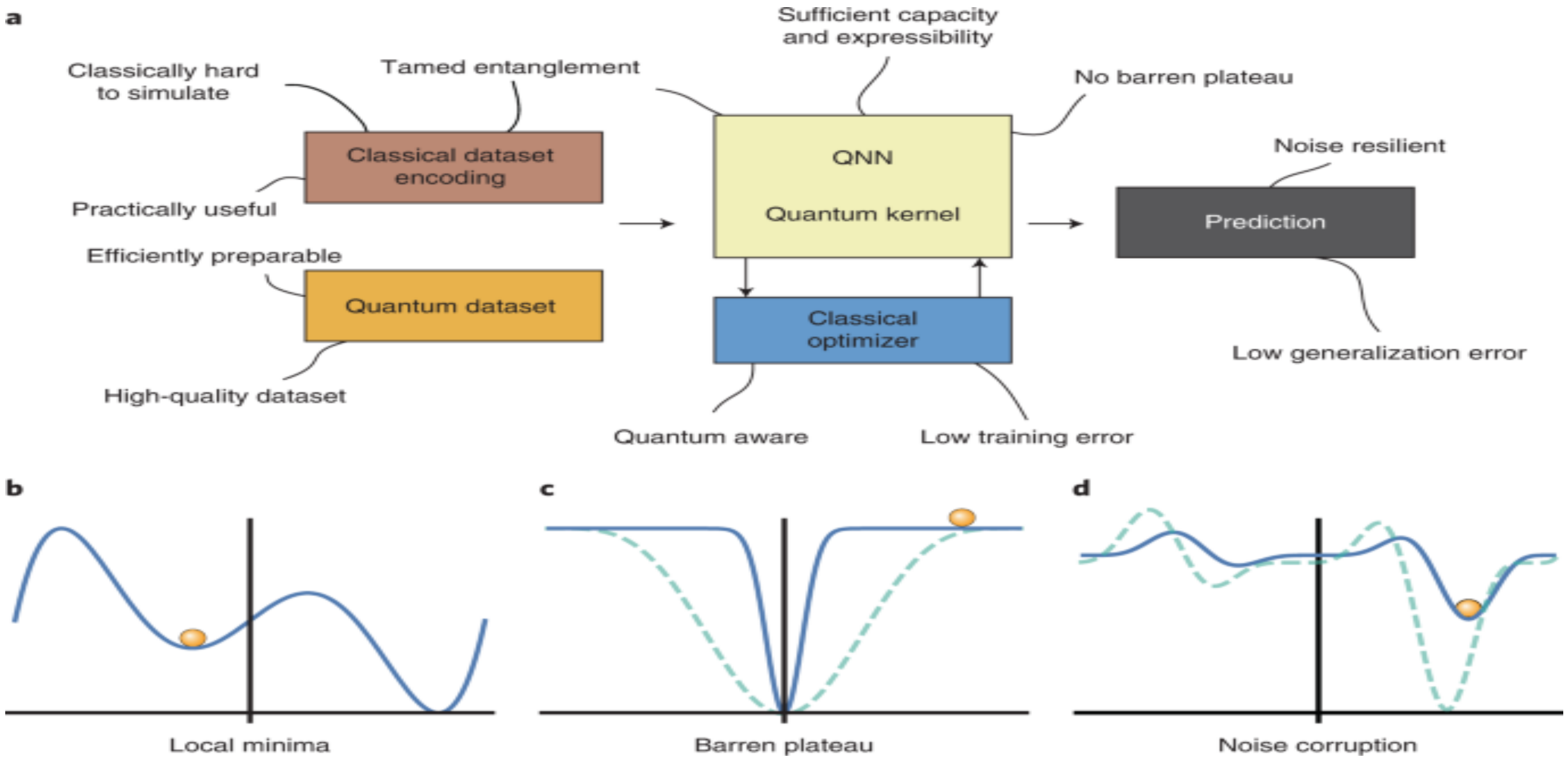


Fidelity circuit

Noise	Squeezed Kernel	Our
0.1	0.825	**0.92**
0.2	0.80	**0.88**
0.2	0.75	**0.86**
1.0	0.65	**0.78**

1. ”Harnessing the power of complex non-linear operator for Quantum Devices,” revision in Nature.
2. Tiwari, Prayag, et al. "Kernel method based on non-linear coherent states in quantum feature space." Journal of Physics A: Mathematical and Theoretical 55.35 (2022): 355301.

Challenges in QML



a) There are several ingredients and priors needed to build a QML model: a dataset (and an encoding scheme for classical data), the choice of parameterized model, loss function, and classical optimizer. In this diagram, we show some of the challenges of the different components of the model.
b-d) The success of the QML model hinges on an accurate and efficient training of the parameters.
However, there are certain phenomena that can hinder QML trainability. These include the abundance of low-quality local minima solutions shown in b), as well as the barren plateau phenomenon in c). When a QML architecture exhibits a barren plateau, the landscape becomes exponentially flat (on average) as the number of qubits increases (seen as a transition from dashed to solid line). The presence of hardware noise has been shown to erase the features in the landscape as well as potentially shift the position of the minima. Here, the dashed (solid) line corresponds to the noiseless (noisy) landscape shown in d).

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Quantum Resources

- Qiskit (https://qiskit.org/ecosystem/machine-learning/index.html)
- Pennylane (https://pennylane.ai/)
- myQLM (https://atos.net/en/lp/myqlm)
- IBM Quantum systems (https://www.ibm.com/quantum/qiskit-runtime) --quantum system with 7-qubit, 5-qubit QPUs, 27-qubit Falcon systems, 127-qubit Eagle systems, or simulators.
- …….

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Thank You!