JAKJOUD LABS
Tech for humanity

Ecole Supérieure d'Informatique et du Numérique
COLLEGE OF ENGINEERING & ARCHITECTURE

Capstone Project

To obtain

Engineering Diploma

Degree specialty of

Computer Engineering – Big Data & Artificial Intelligence

Evaluating Classical and Quantum Hybrid Approaches for Breast Cancer Diagnosis: A Performance Comparison

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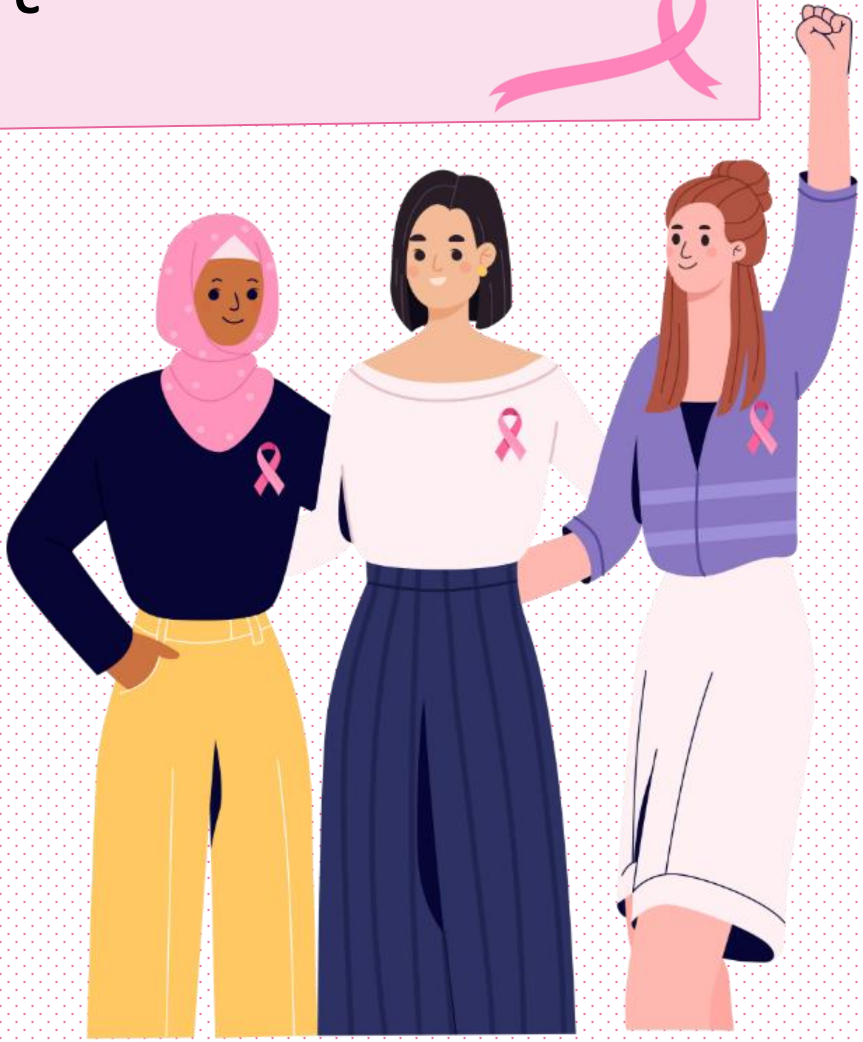
Wed 05 June 2024

بِسْمِ ٱللَّهِ ٱلرَّحْمَٰنِ ٱلرَّحِيمِ

Table of Content



Introduction

Breast cancer is a leading cause of death among women worldwide, making early and accurate diagnosis essential for effective treatment. This project investigates the combination of classical machine learning and quantum computing techniques.

II. Context & Motivation

Presentation of the Hosting Organization: Synergeon

- **Founded**: September 2020 by Mr. Karim Amor.
- **Location:** Casablanca, Morocco
- **Specialization**: Robotics, software, IoT, AI, and blockchain (NFT) solutions.
- **Mission:** Focus on "Moonshot projects" with massive societal impact using cutting-edge technologies.

Presentation of the Contracting Laboratory: Jakjoud Labs

- **Founded**: 2022 by Abdeslam, Widad, Hicham, and Fatima Zohra Jakjoud.
- **Location:** Marrakech, Morocco.
- **Specialization:** Engineering of computer solutions, Cloud solution architectures, Engineering of embedded systems, AI and data science, Quantum Computing…
- **Special Features:** Stakeholder in the Moroccan quantum computer project (first in Africa).

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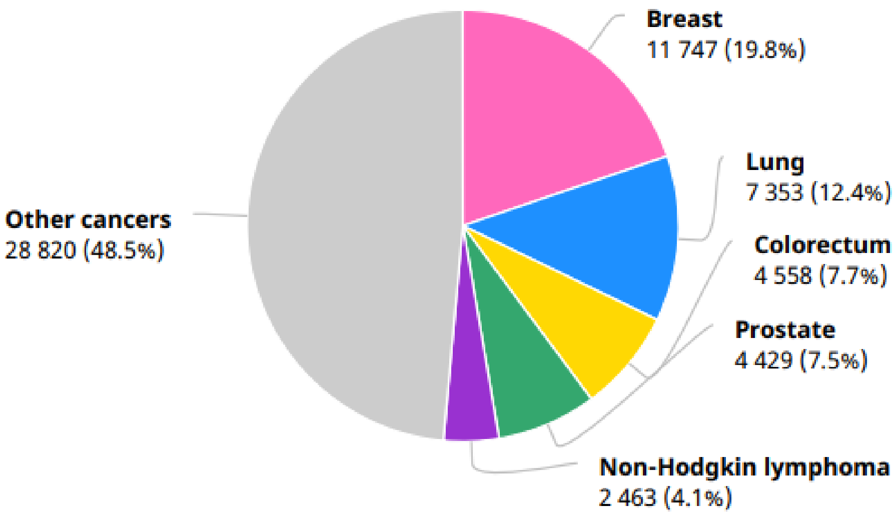
International Agency for Research on Cancer
World Health Organization

Morocco
Source: Globocan 2020

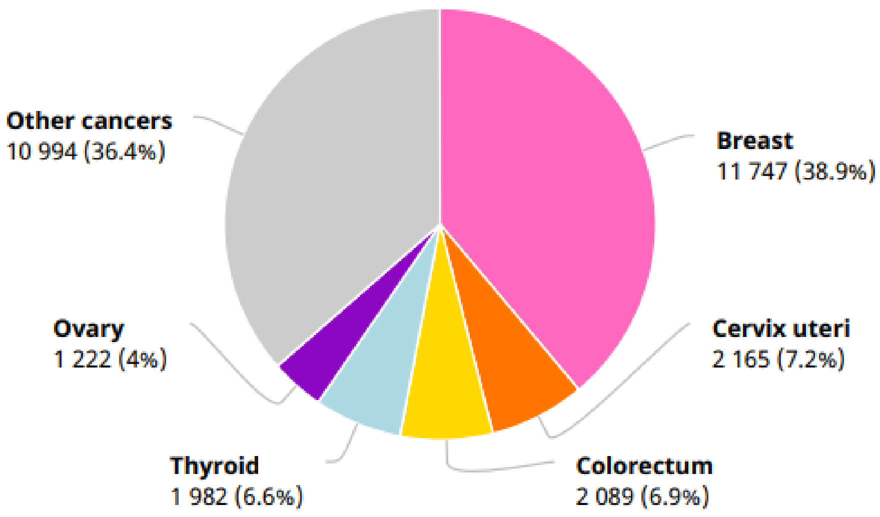
Breast Cancer in Morocco

Number of new cases in 2020, both sexes, all ages



Total: 59 370

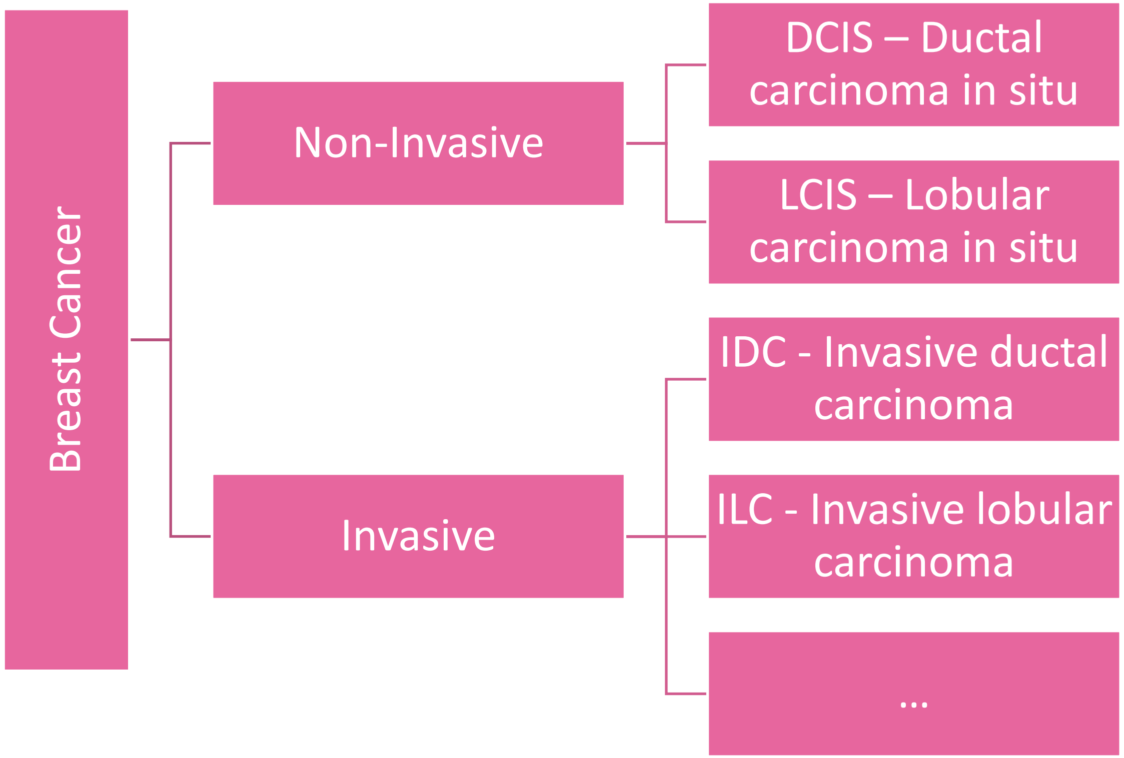
Number of new cases in 2020, females, all ages

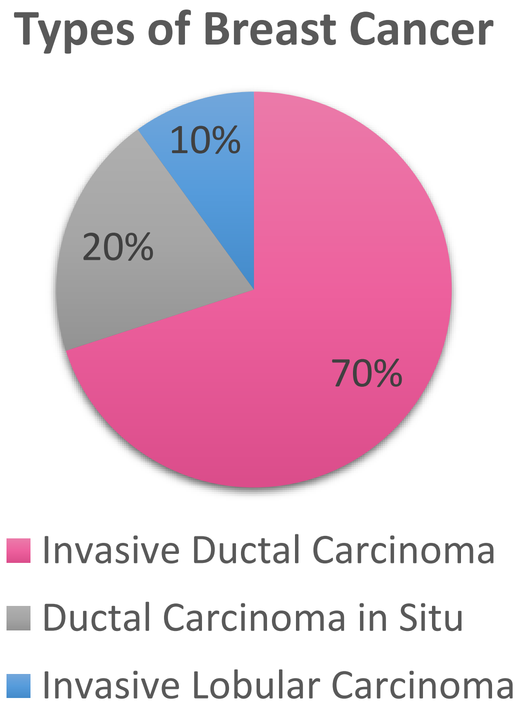


Total: 30 199

2. Context & Motivation

Breast Cancer Types





Motivations

High Prevalence and Mortality.

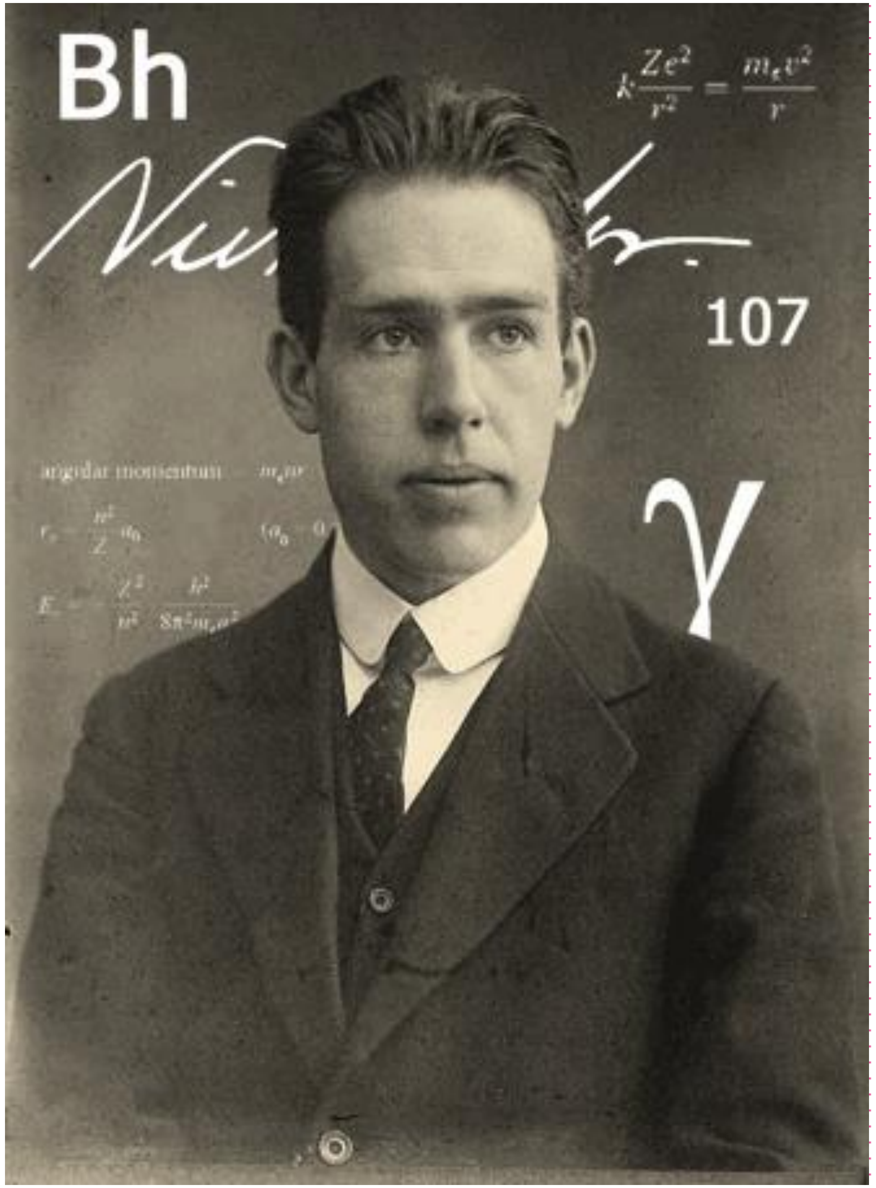
Rising Incidence in Morocco.

Limitations of Current Detection Methods.

Potential of Quantum Computing.

Advancing Medical Diagnostic.

3. Quantum Computing



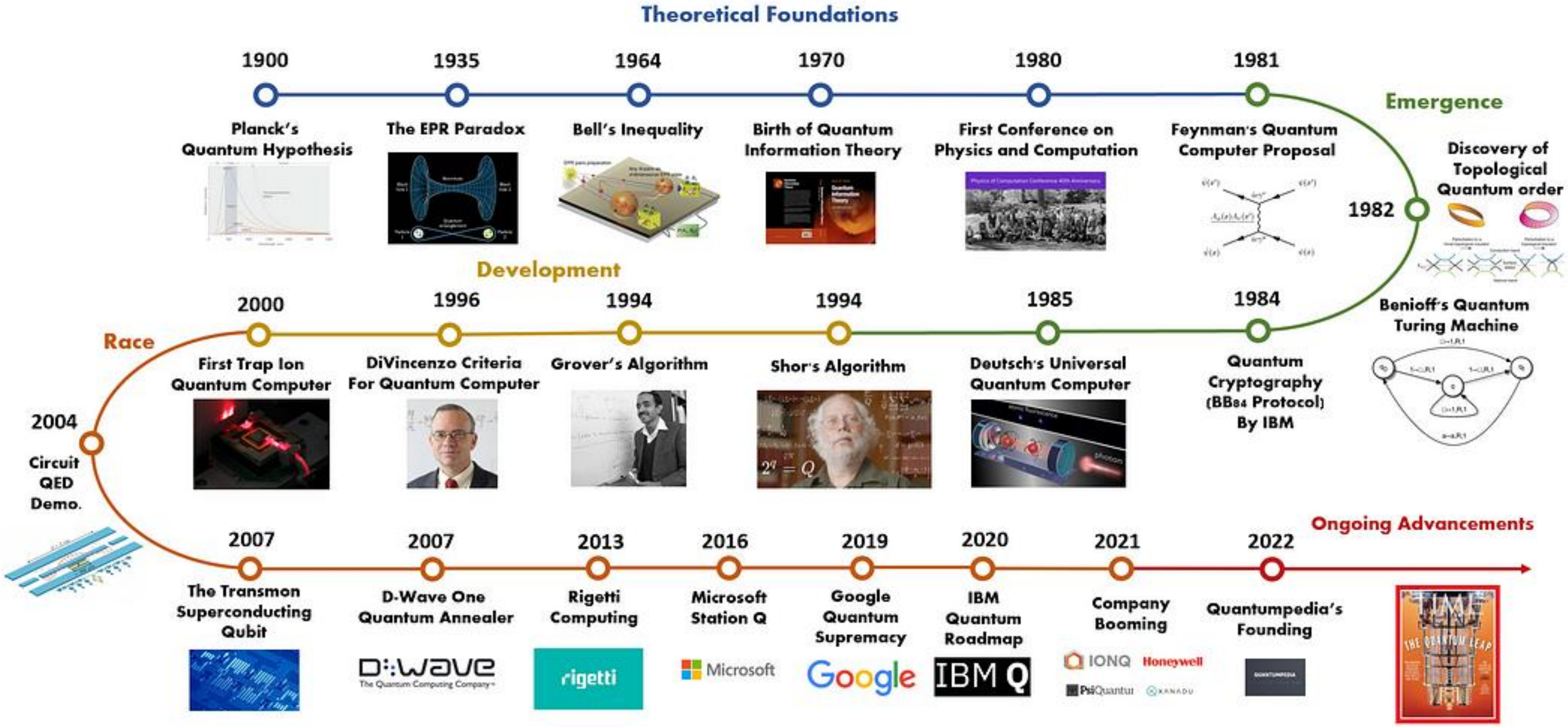
3. Quantum Computing

"Anyone who can contemplate quantum mechanics without getting dizzy hasn't understood it."

Niels Bohr

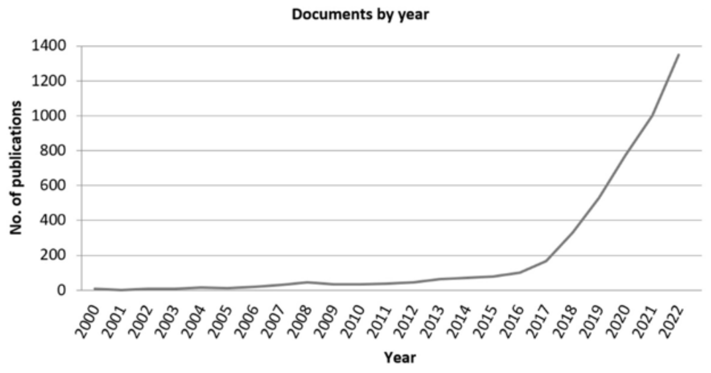
3. Quantum Computing

Timeline progression of Quantum Computing milestones

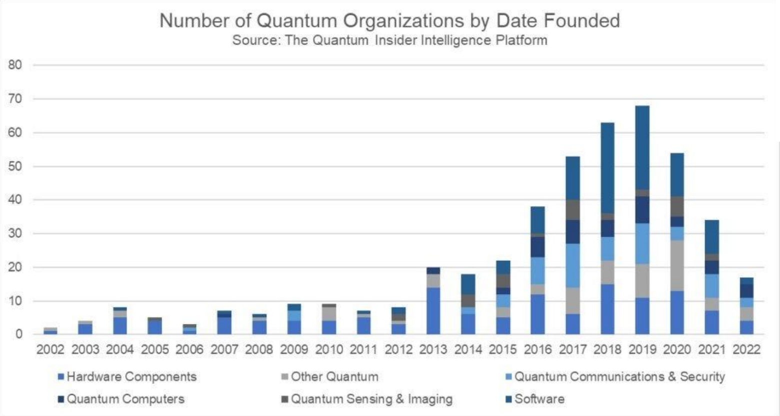


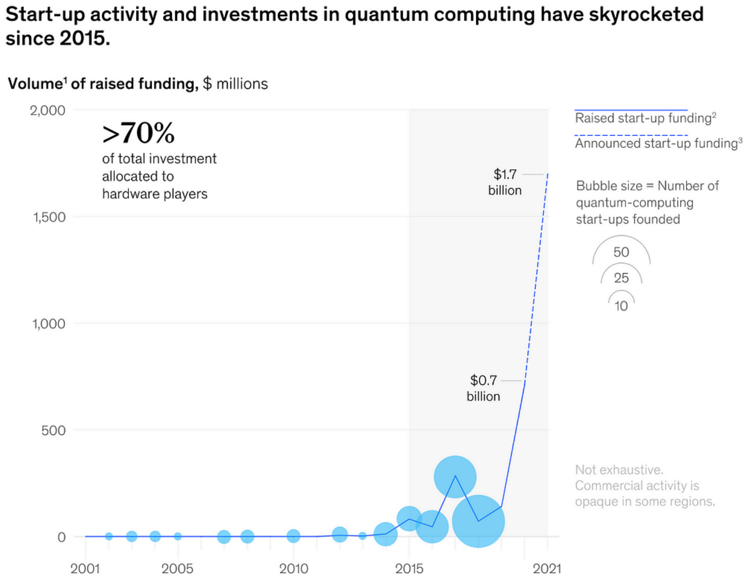
3. Quantum Computing

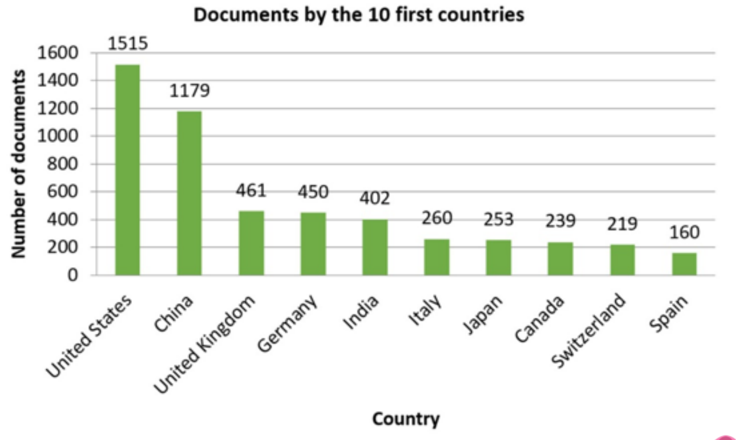
Timeline progression of Quantum Computing milestones



Number of relevant publications per year about QML (Statistics March 2023).

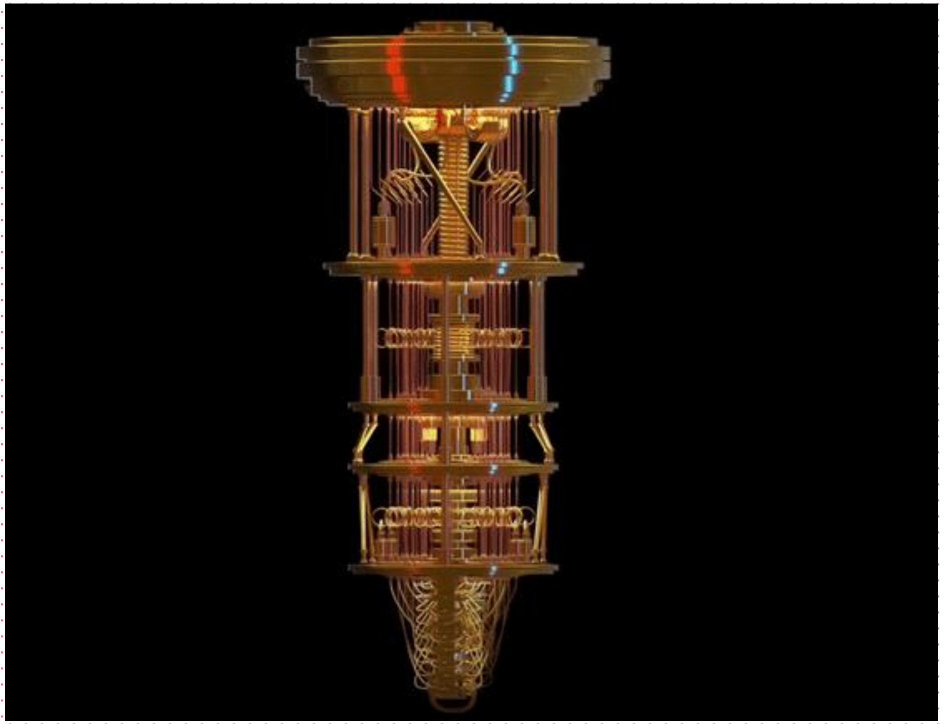






Countries that have published (Scopus source) papers related to QML.

3. Quantum Computing



Important Definitions

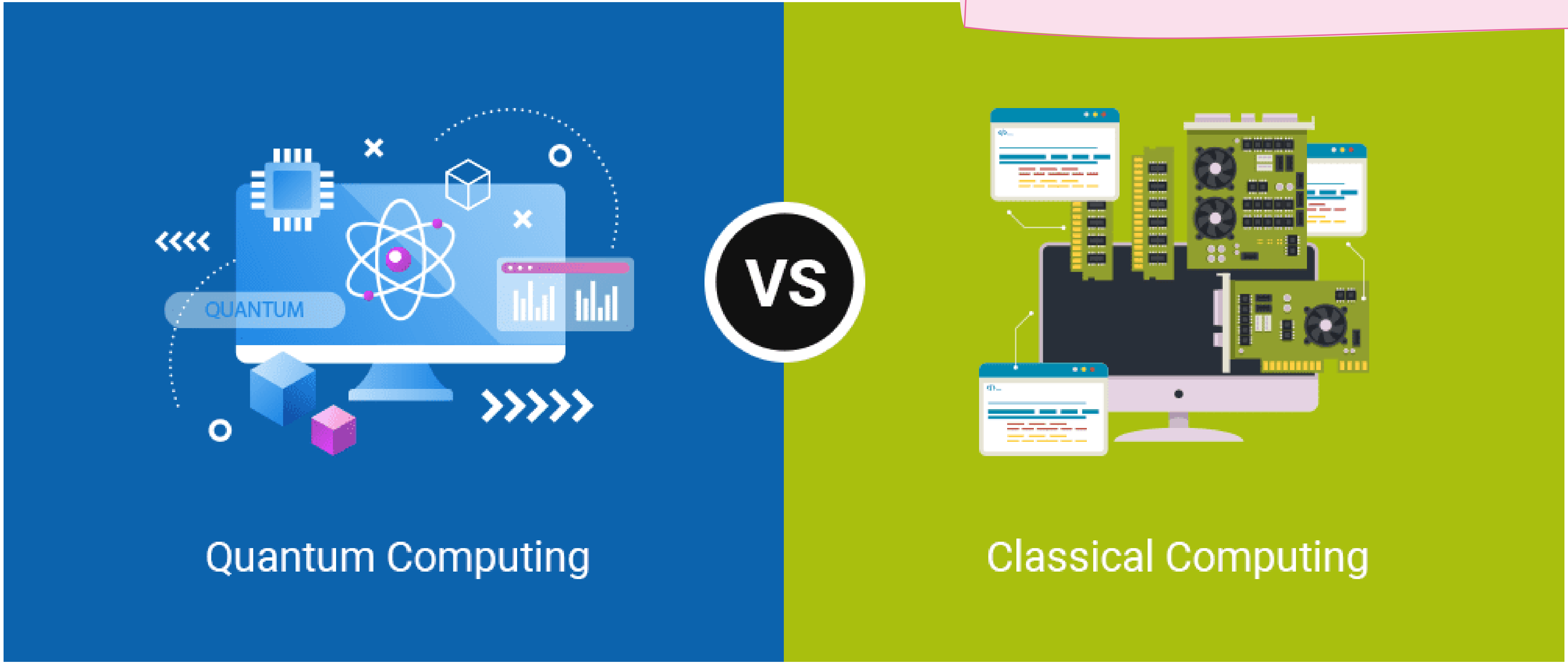
What does “Quantum” mean?

"Quantum" refers to the smallest possible amount of a physical quantity involved in an interaction, according to quantum theory.

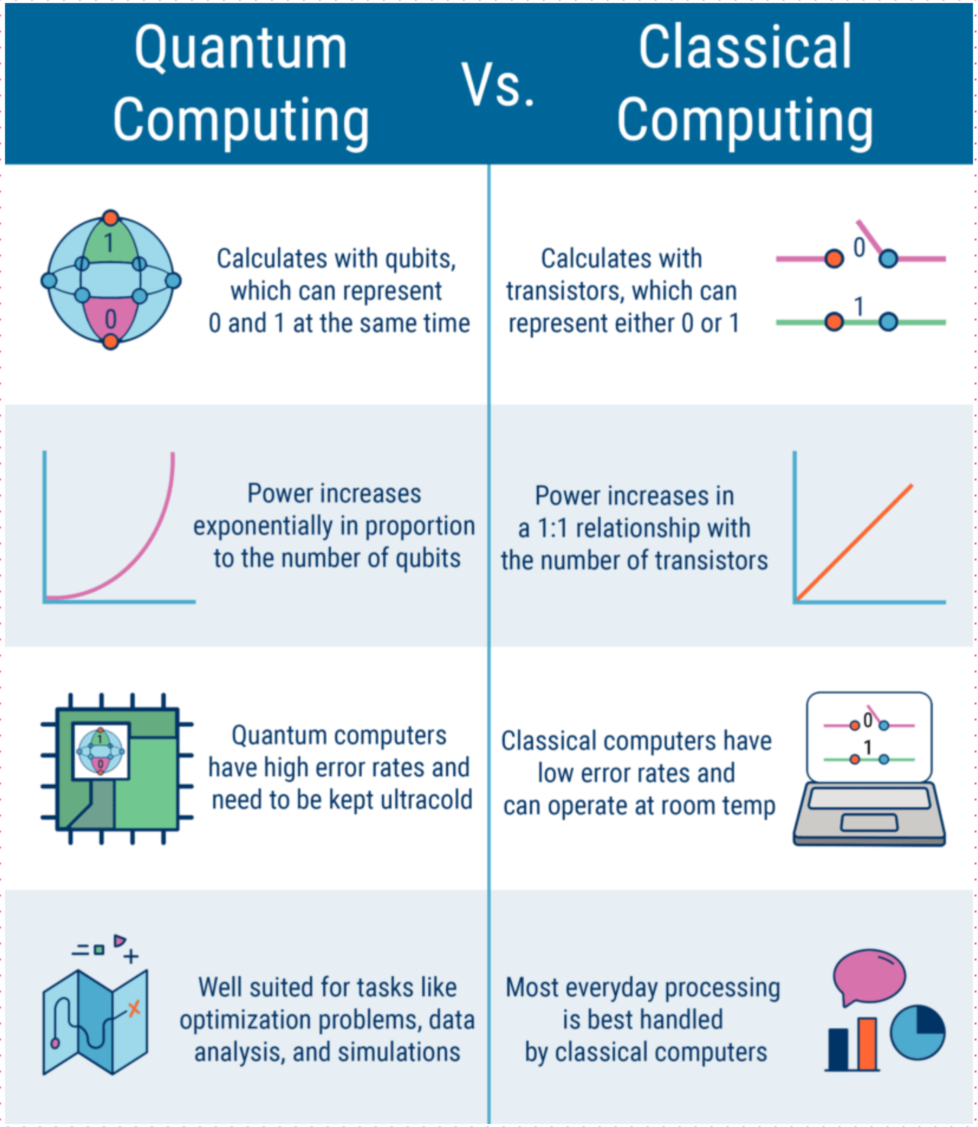
What is a “Quantum Computer”?

A quantum computer is a machine that performs calculations based on the laws of quantum mechanics, which is the behavior of particles at the sub-atomic level.

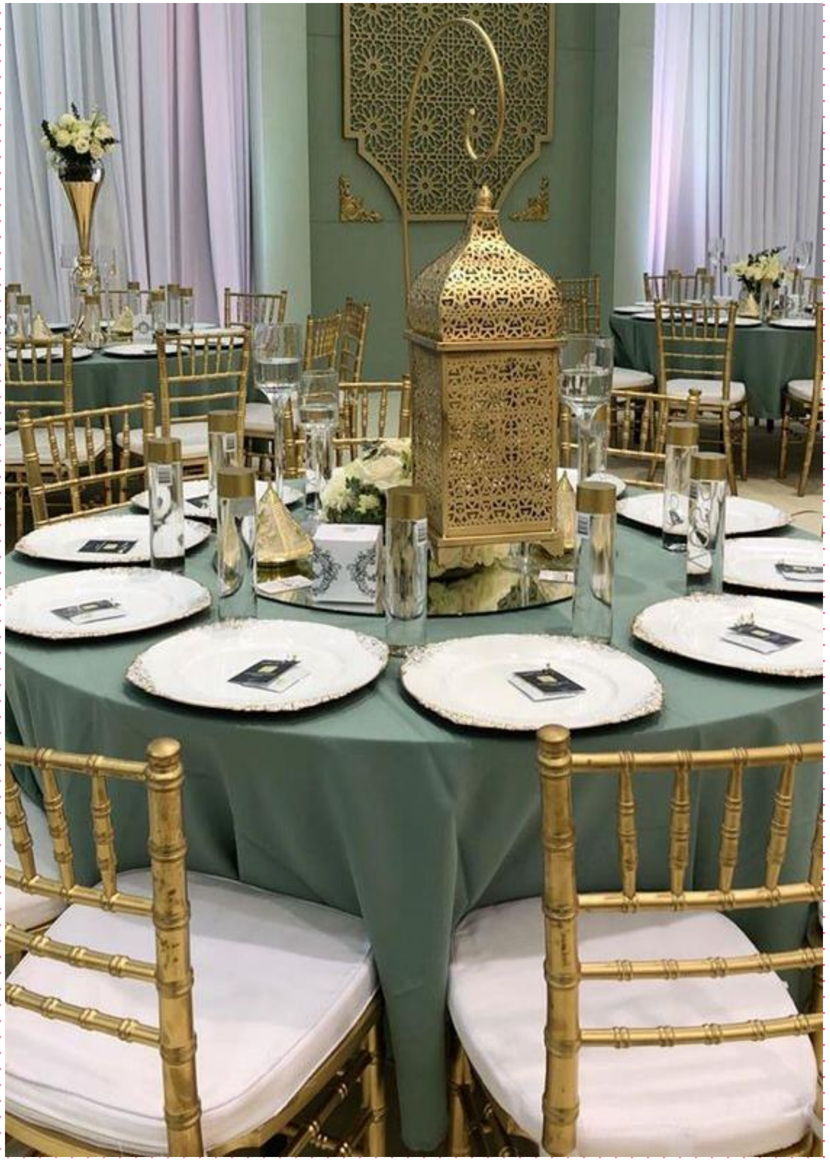
3. Quantum Computing



3. Quantum Computing



Classical computers excel in *sequential processing* and *deterministic algorithms*, while quantum computers offer the potential for *exponential speedup* in *parallel processing* and *probabilistic computations*.



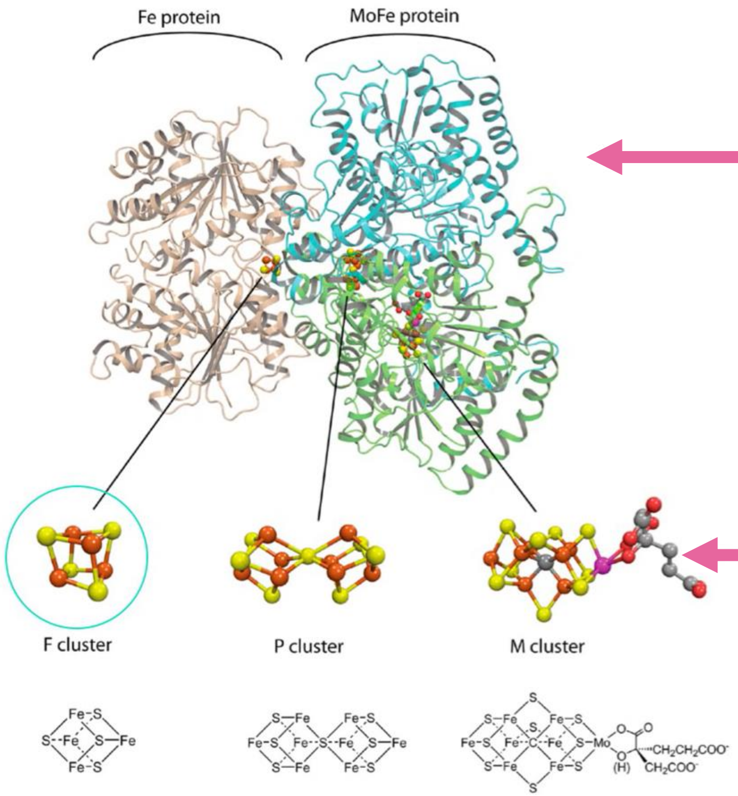
3. Quantum Computing

Two Facts:

Fact 1: Classical Computers have enabled amazing things.

Fact 2: There are still problems we just can't solve.

Chemistry



Simulating this cluster is at the **limit** of classical computers

Nitrogenase enzyme involved in **N_2 to NH_4**

Reaction.

These regions are involved in different reaction stages.

Iron sulfide clusters (**Fe_x S_y**) of **different sizes**

What do these problems have in common?

3. Quantum Computing

Rice and chessboard problem

If you started with one grain of rice on the 1st square of a chessboard, doubled it on the 2nd, and kept doubling on each square, how much rice would you have?

A. 1,024 grains of rice
B. 65,536 grains of rice
C. 4,294,967,296 grains of rice
D. 18,446,744,073,709,551,616 grains of rice

Rice and chessboard problem

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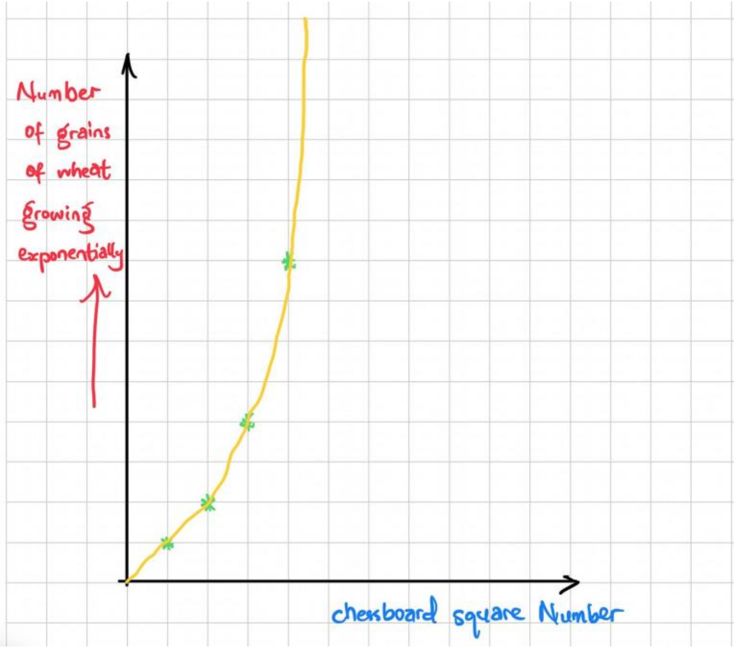
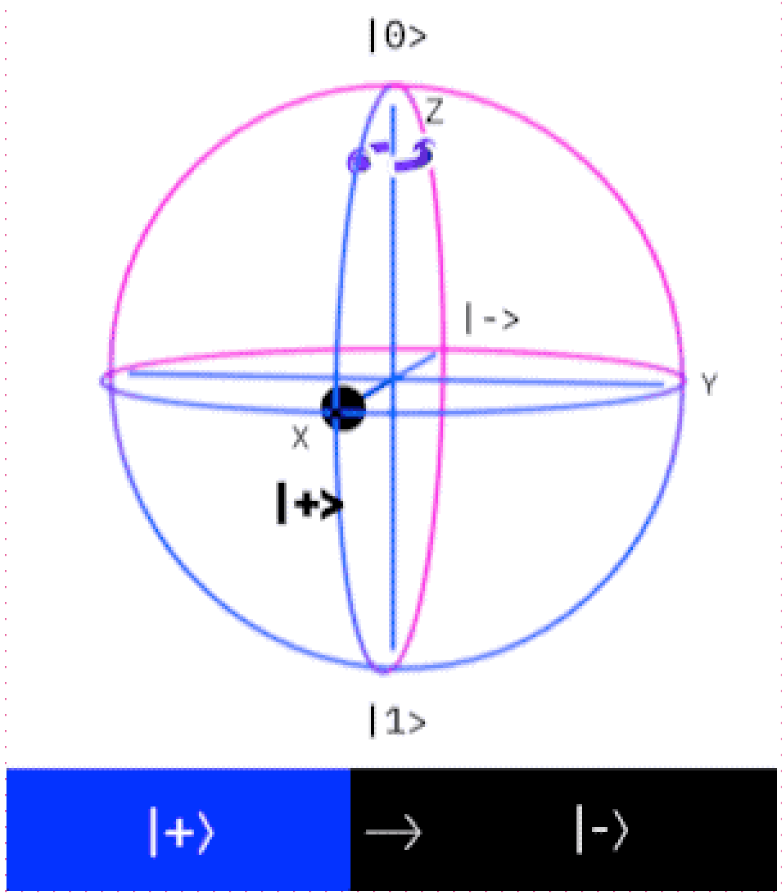


Answer: D. $2^{64}-1$ grains of rice

3. Quantum Computing

Representation of Data - Qubits

- A qubit (or quantum bit) is the quantum mechanical analogue of a classical bit.
- In quantum computing the information is encoded in qubits.
- A qubit is a two-level quantum system where the two basis qubit states are usually written as $|0\rangle$ and $|1\rangle$.

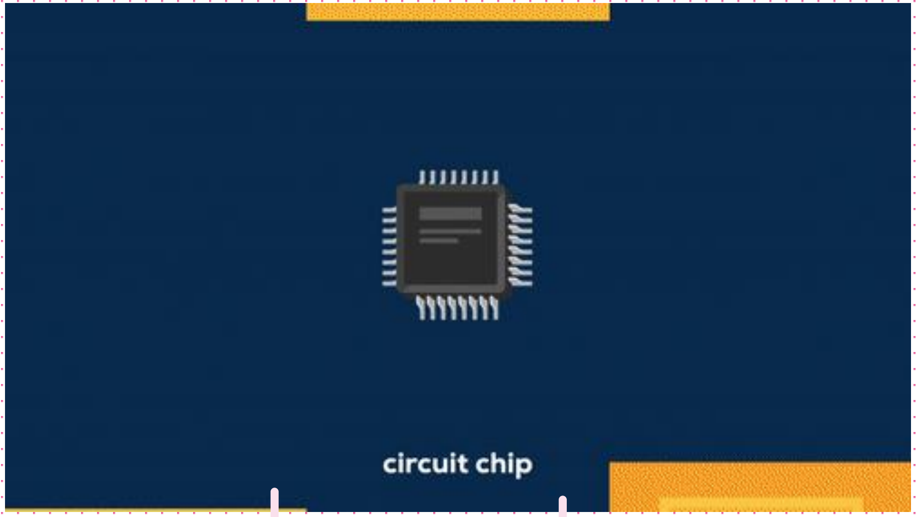


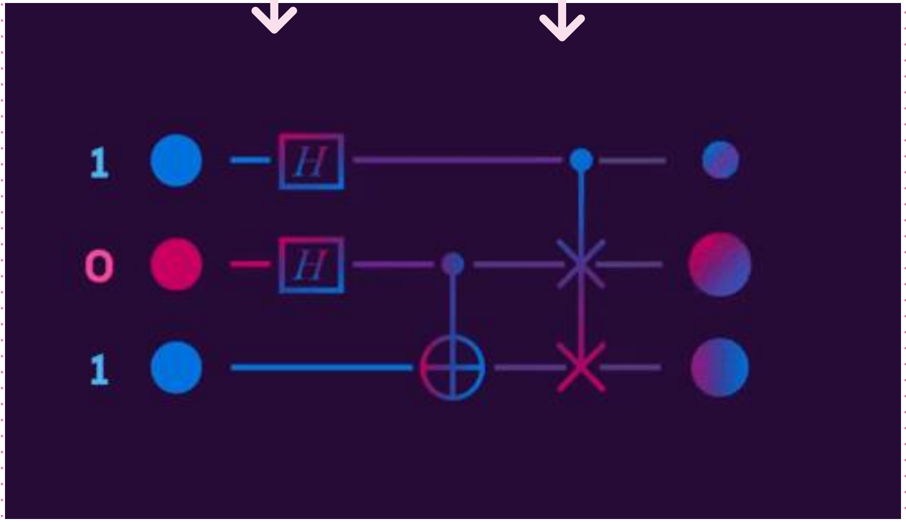
3. Quantum Computing

Visualization

- **Bloch Sphere:**
    - A common way to visualize qubits is the Bloch sphere, a 3D representation of a qubit's state.
    - The north and south poles represent |0⟩ and |1⟩, while any point on the sphere represents a possible superposition state.

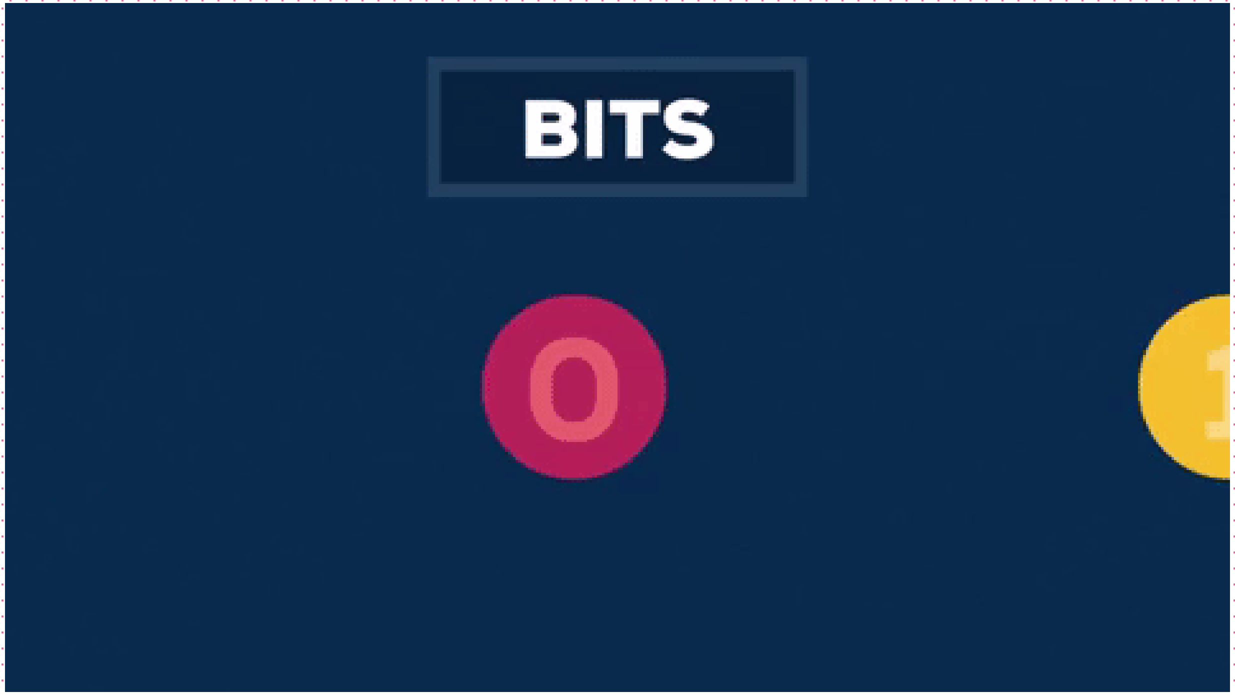
3. Quantum Computing





Quantum Circuits

- Quantum circuits are the quantum computing equivalent of classical logic circuits, consisting of a series of quantum gates applied to qubits.
- Key gates include the Hadamard gate (creates superposition), the CNOT gate (creates entanglement), and the Pauli-X gate (quantum equivalent of the classical NOT gate)..



3. Quantum Computing

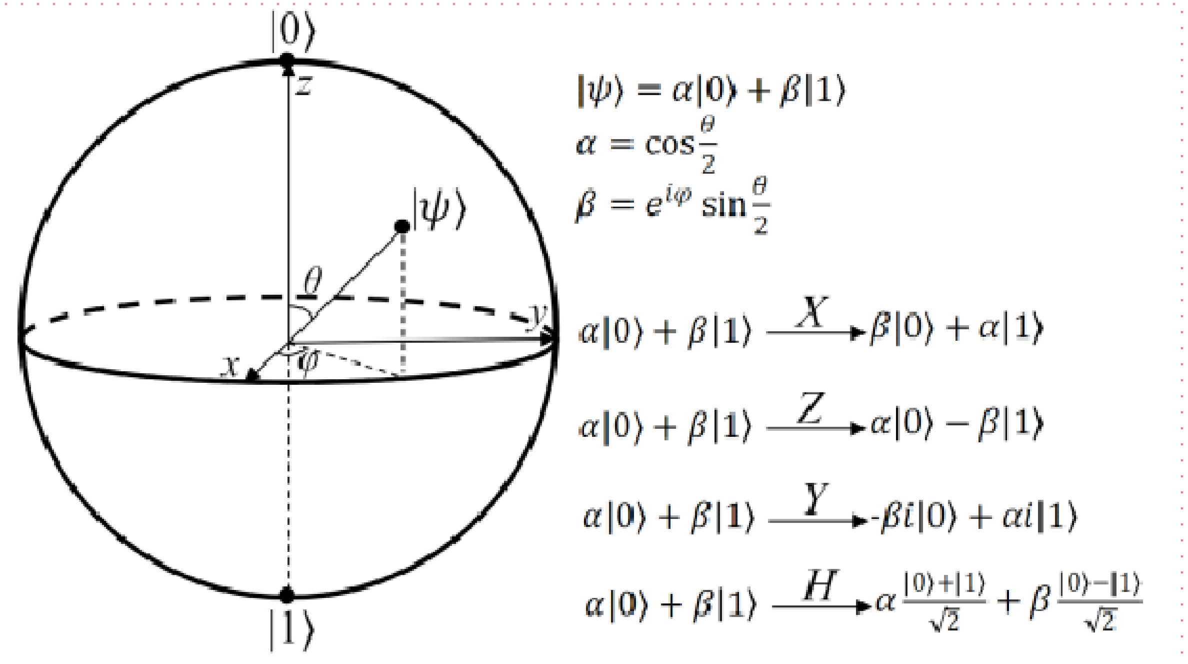
Superposition

- Superposition is a fundamental principle of quantum mechanics where a qubit can exist in a combination of both $|0\rangle$ and $|1\rangle$ states simultaneously.
- This allows quantum computers to process multiple possibilities at once, enabling parallelism in computations..
- A general -pure- qubit state is expressed as:

$$\psi = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} ; |\alpha| + |\beta| = 1$$

where α and β are the complex probability amplitudes for each basis state

3. Quantum Computing



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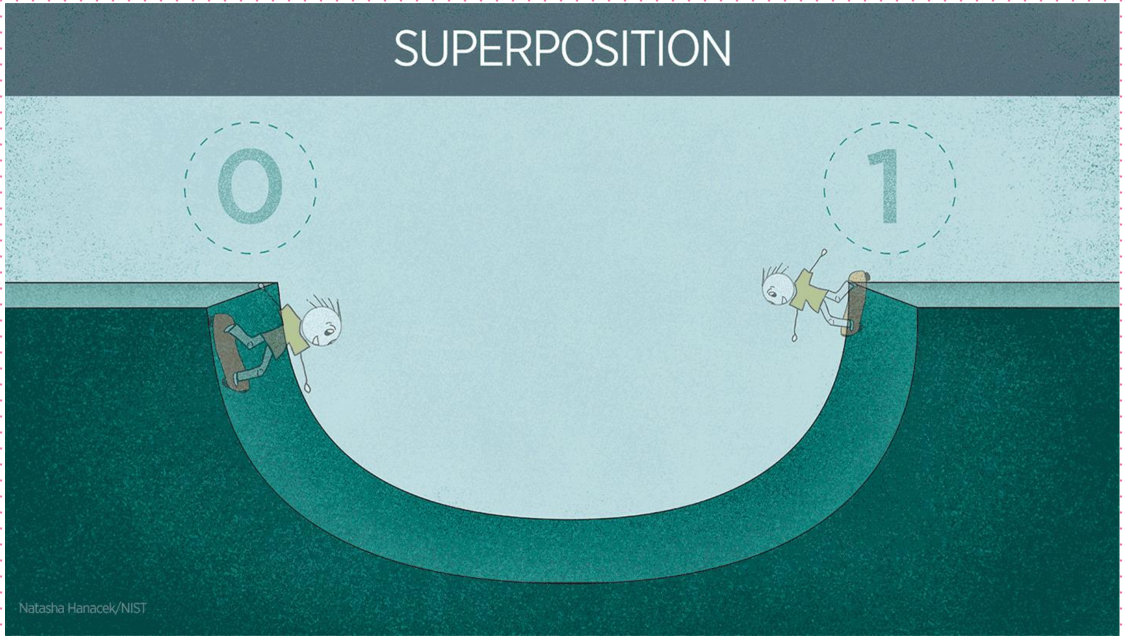

3. Quantum Computing

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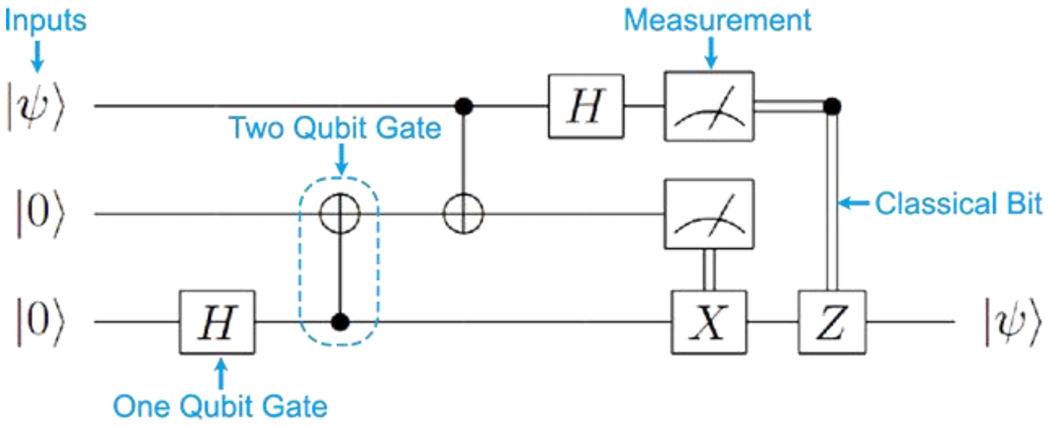
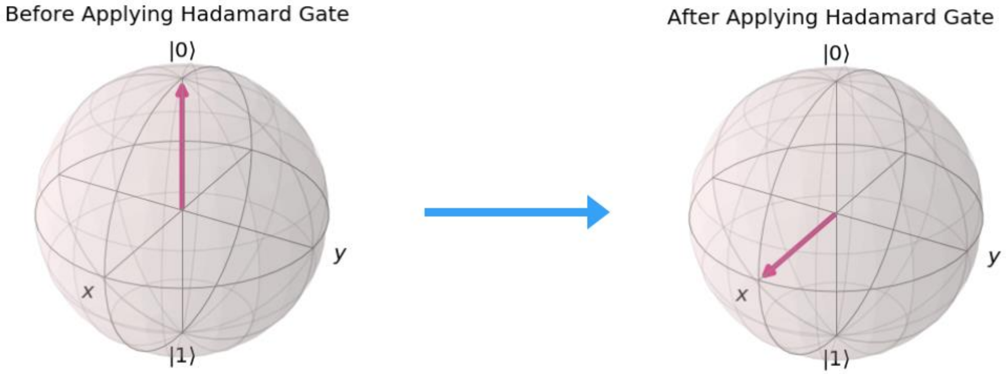
Putting a Qubit in Superposition Using the Hadamard Gate

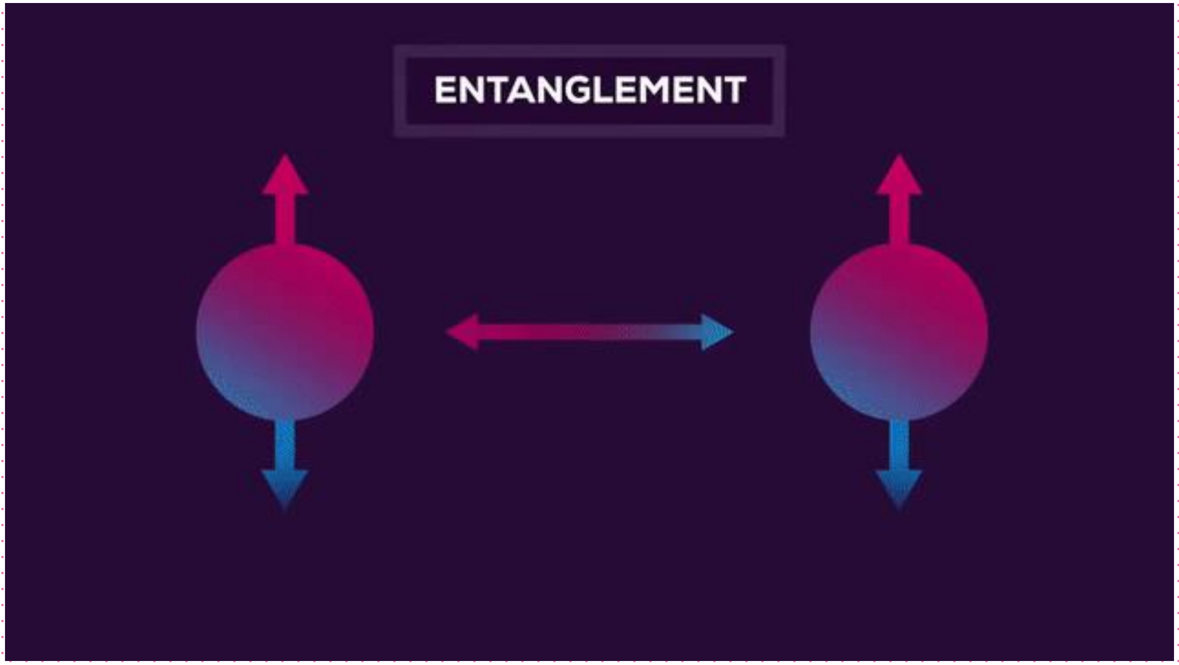
- Initial State is |0⟩ represented as a column vector: $|0\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- Applying the Hadamard Gate: $H: = \frac{1}{\sqrt{2}} \begin{matrix} 1 & 1 \\ 1 & -1 \end{matrix}$

→ The qubit is now in a superposition state:

$$H\,|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \times 1 + 1 \times 0 \\ 1 \times 1 + -1 \times 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



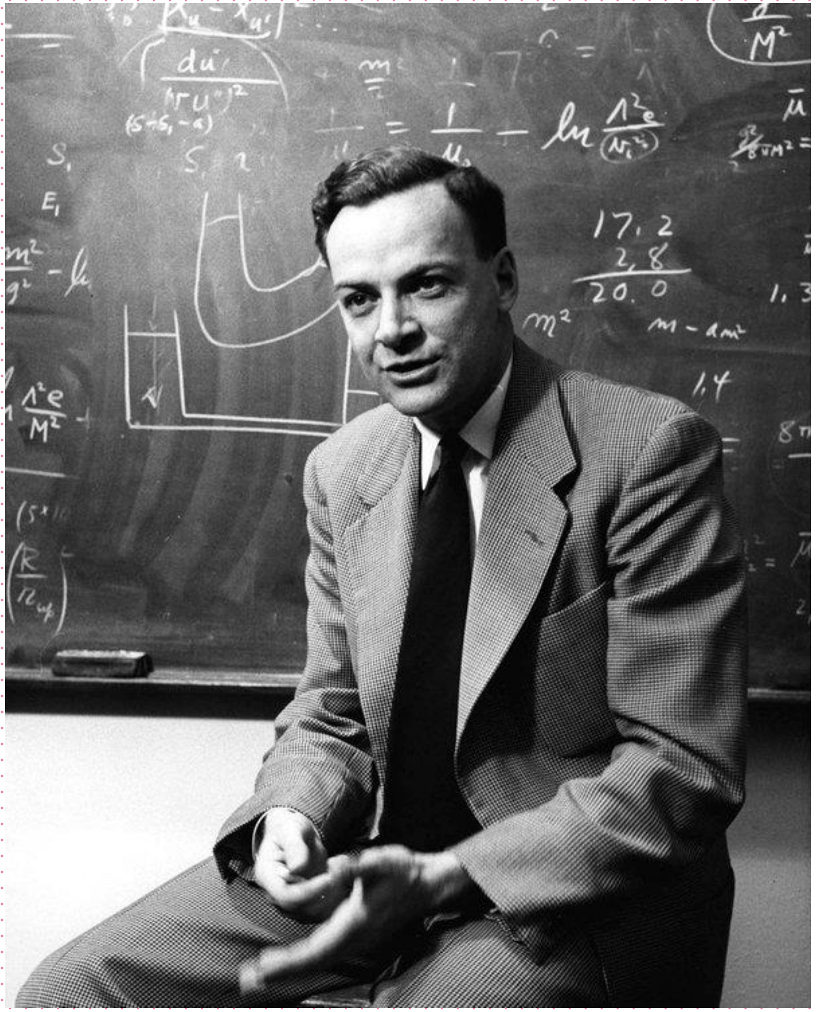




3. Quantum Computing

Relationship between Data - Entanglement

- Entanglement is a quantum phenomenon where qubits become interconnected and the state of one qubit instantly affects the state of another, no matter the distance.
- For two entangled qubits, their combined state might be expressed as $\psi = \alpha|00\rangle + \beta|11\rangle$, indicating a correlation between the states.



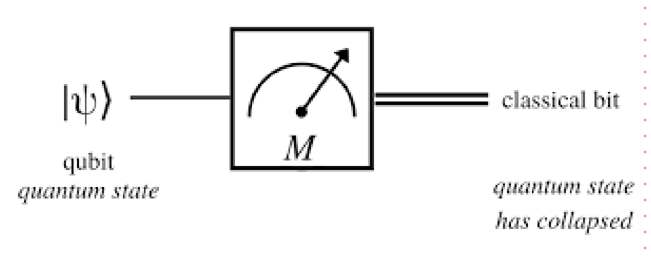
3. Quantum Computing

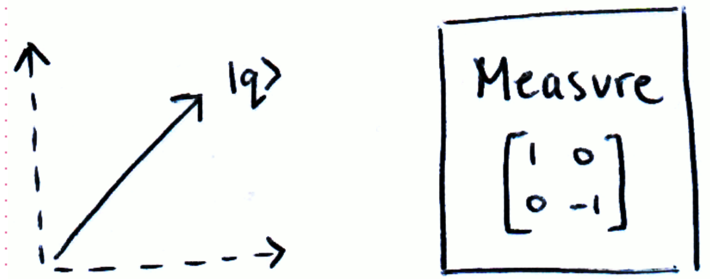
"I think I can safely say that nobody understands quantum mechanics."

Richard Feynman

3. Quantum Computing

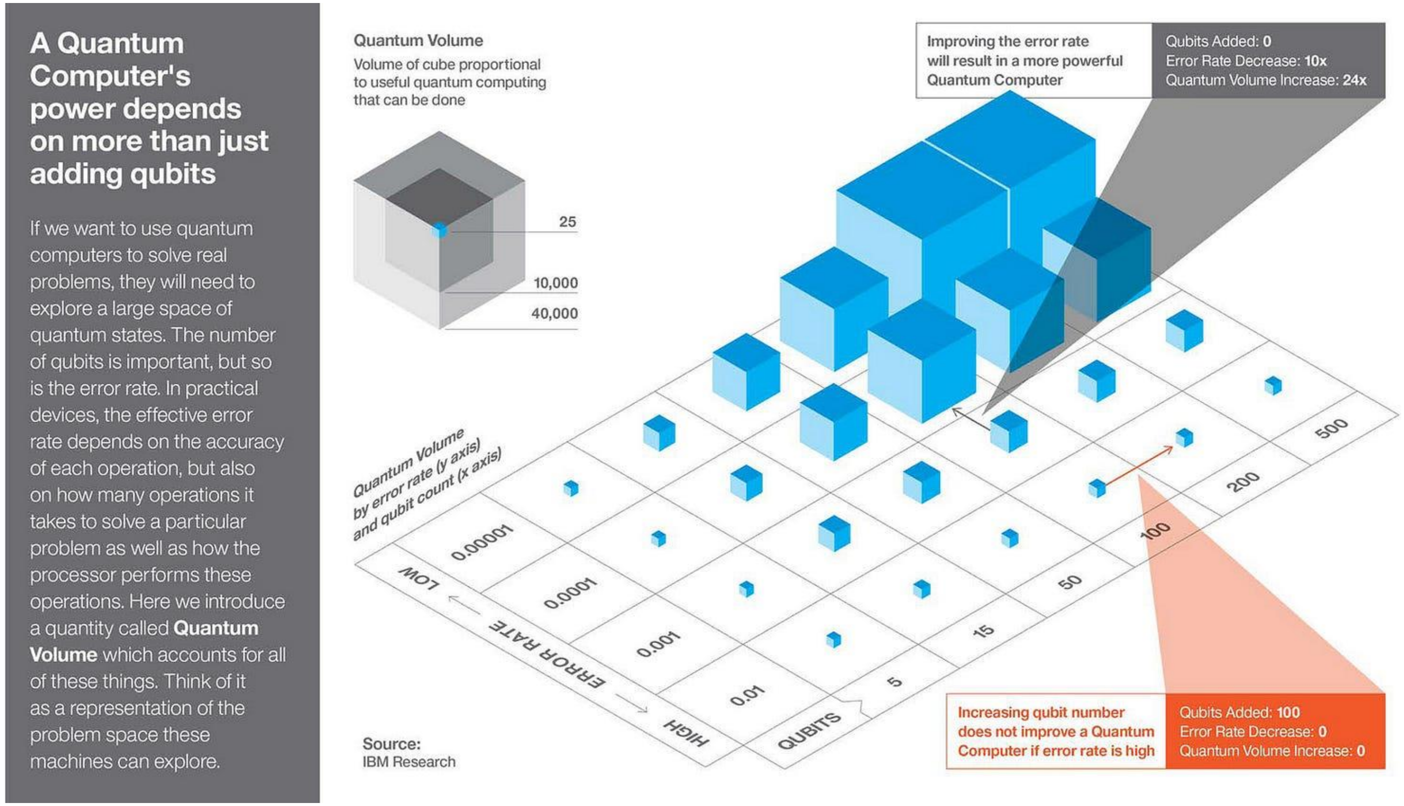
Data Retrieval - Measurement

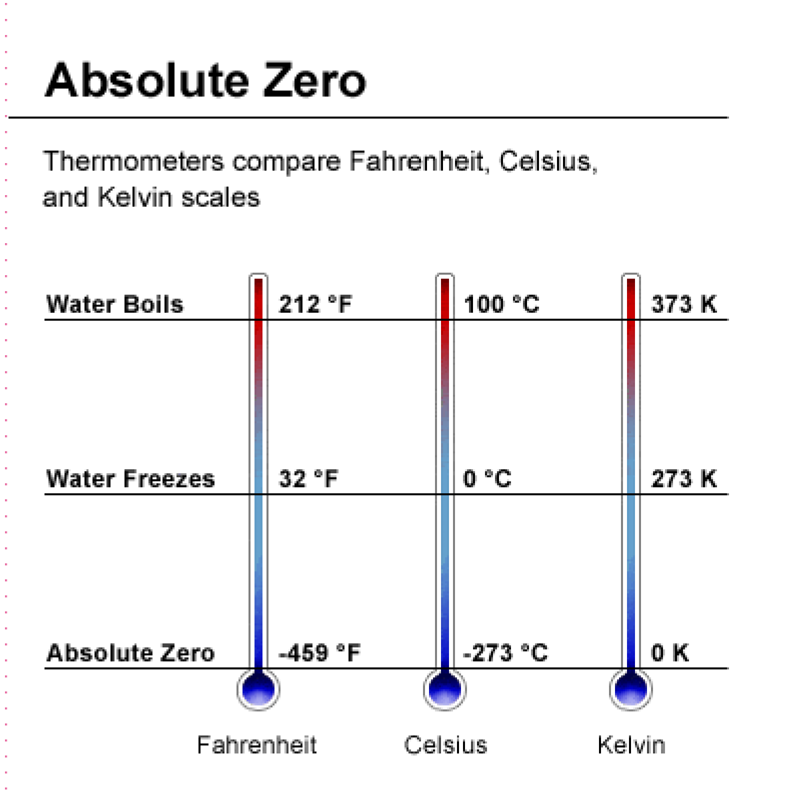




- Measurement in quantum computing collapses a qubit's superposition state to one of the basis states (|0⟩ or |1⟩).
- The outcome of the measurement is probabilistic, determined by the magnitudes of α and β.
- Measurement disrupts the quantum state, meaning the superposition is lost, and only a definite state is observed.

Roadblocks awaiting breakthroughs





3. Quantum Computing

Challenges in Quantum Computing:

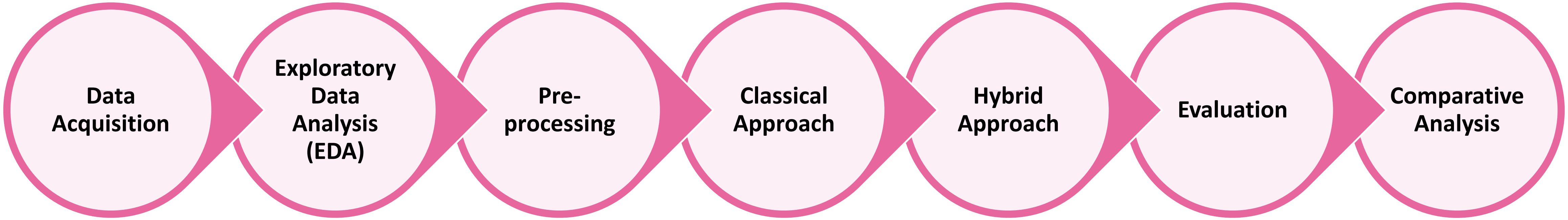
Decoherence : the loss of quantum coherence, where quantum states lose their quantum properties due to interaction with the environment.

Construction Costs:

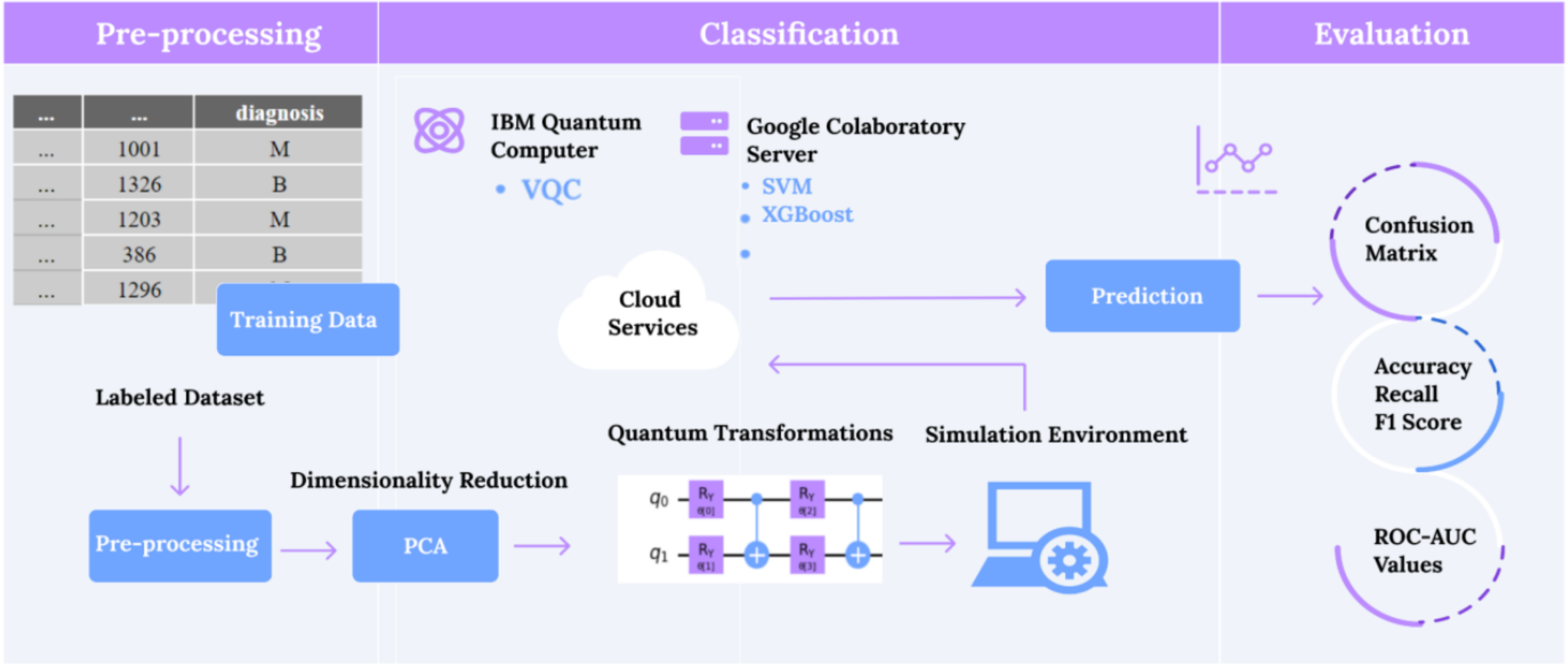
- Specialized Hardware: Quantum processors require materials like superconductors, topological insulators, or trapped ions.
- Cryogenic Systems: Essential for maintaining qubits at extremely low temperatures (near absolute zero) to reduce decoherence.

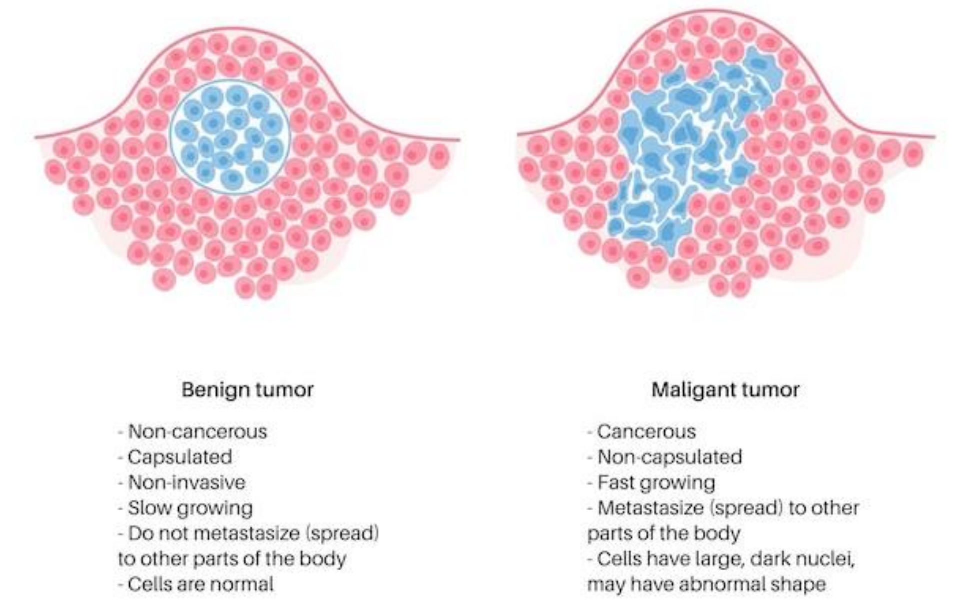
IV. Methodology

4. Methodology



4. Methodology





Number	Attributes
1	ID number
2	Diagnosis (M = malignant, B = benign)
3-32	ten real-valued features are computed for each cell nucleus:
a)	Radius (mean of distances from center to points on the perimeter)
b)	Texture (standard deviation of gray-scale values)
c)	Perimeter
d)	Area
e)	Smoothness (local variation in radius lengths)
f)	Compactness (perimeter^2 / area - 1.0)
g)	Concavity (severity of concave portions of the contour)
h)	Concave points (number of concave portions of the contour)
i)	Symmetry
j)	Fractal dimension ("coastline approximation" -1)

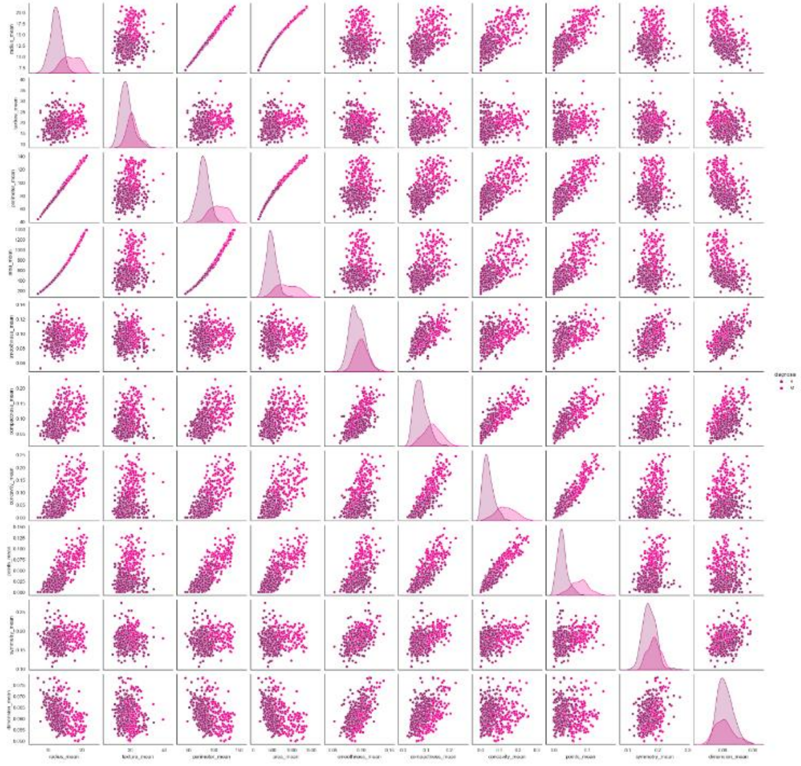
4. Methodology

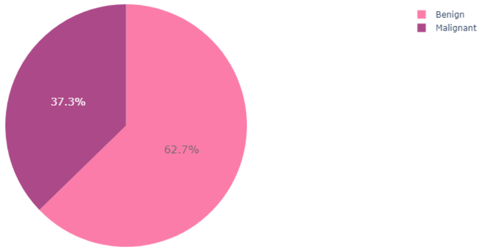
1. Data Acquisition

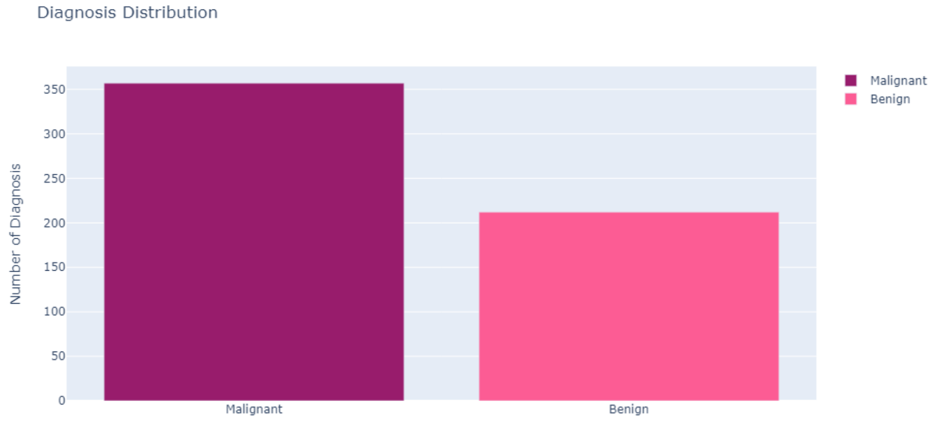
- **Dataset**: Breast Cancer (Wisconsin) Diagnosis dataset from UCI Machine Learning Repository.
- **Features**: 30 features related to cell nuclei characteristics in digitized images from FNAs.
- **Source**: Collected from University of Wisconsin Hospitals, Madison

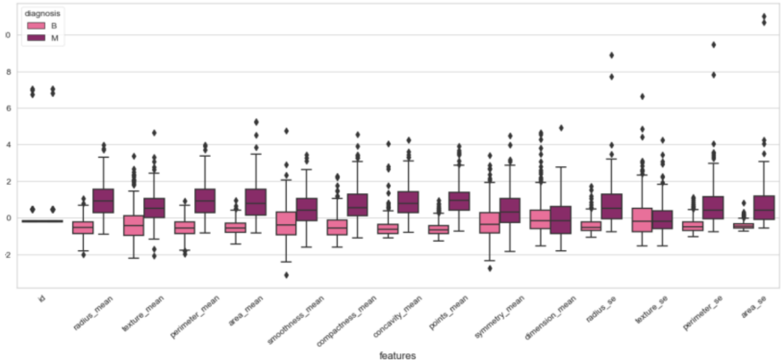
4. Methodology

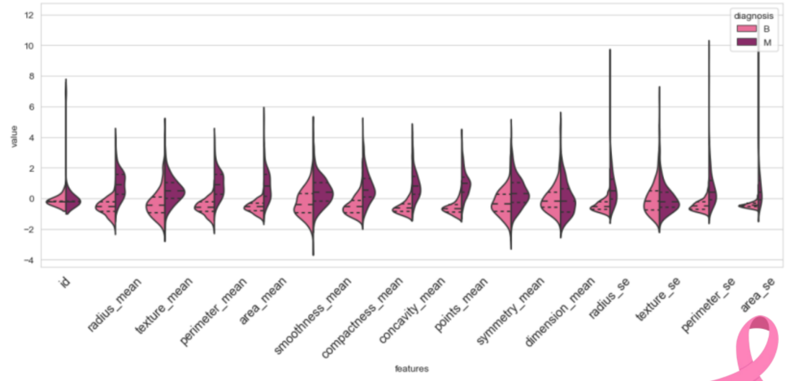
2. Exploratory Data Analysis (EDA)











4. Methodology

3. Pre-processing

- Preprocessing serves as a critical initial phase in any data analysis or modeling task.
  - Remove any duplicate entries to ensure data accuracy and prevent biases.
  - Remove any duplicate entries
  - Standardize features to have a mean of 0 and a standard deviation of .

Check for null and missing values

```
null_values = df.isnull().values.any()
if null_values == True:
    print("There are some missing values in data")
else:
    print("There are no missing values in the dataset")
```

```
There are no missing values in the dataset
```

Check for duplicate elements

```
sum(df.duplicated())
```

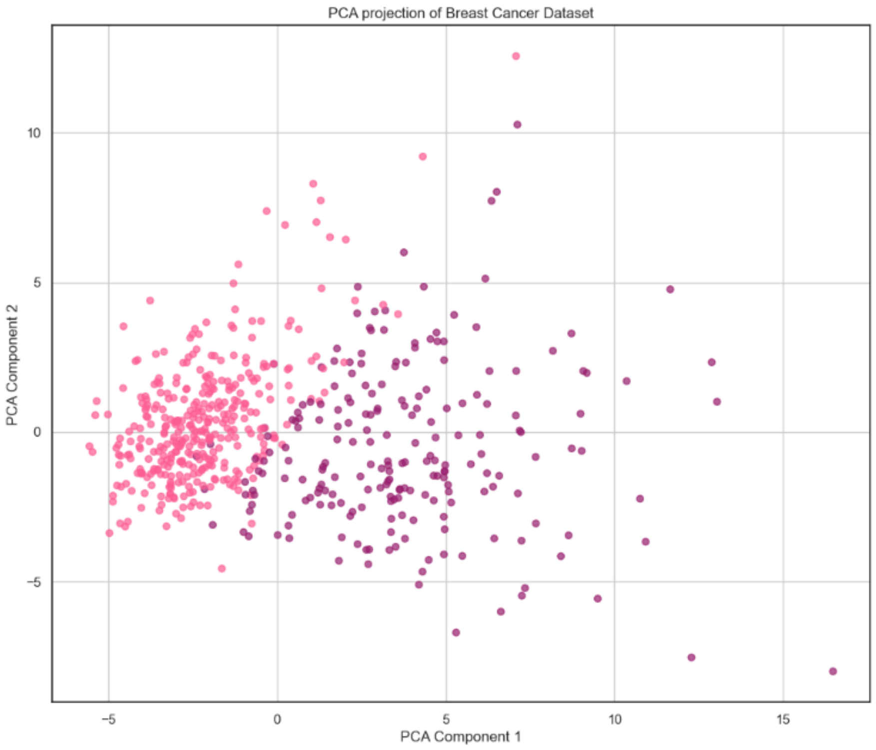
```
0
```

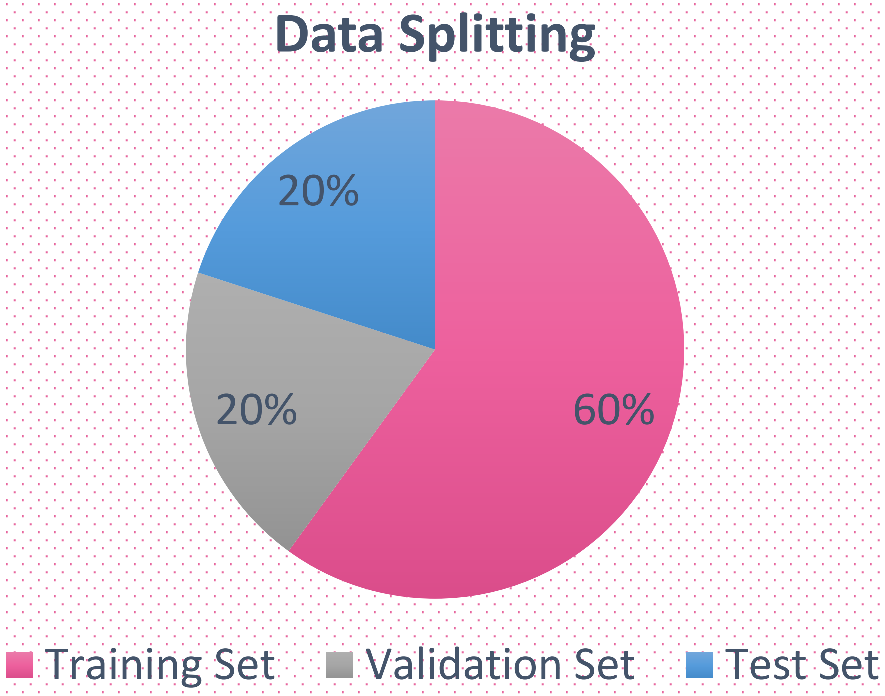
```
X = df.drop('diagnosis',axis=1).values
y = df['diagnosis'].values

sc = StandardScaler()
X = sc.fit_transform(X)
```

$$z = \frac{x - \mu}{\sigma}$$

4. Methodology

Dimensionality Reduction





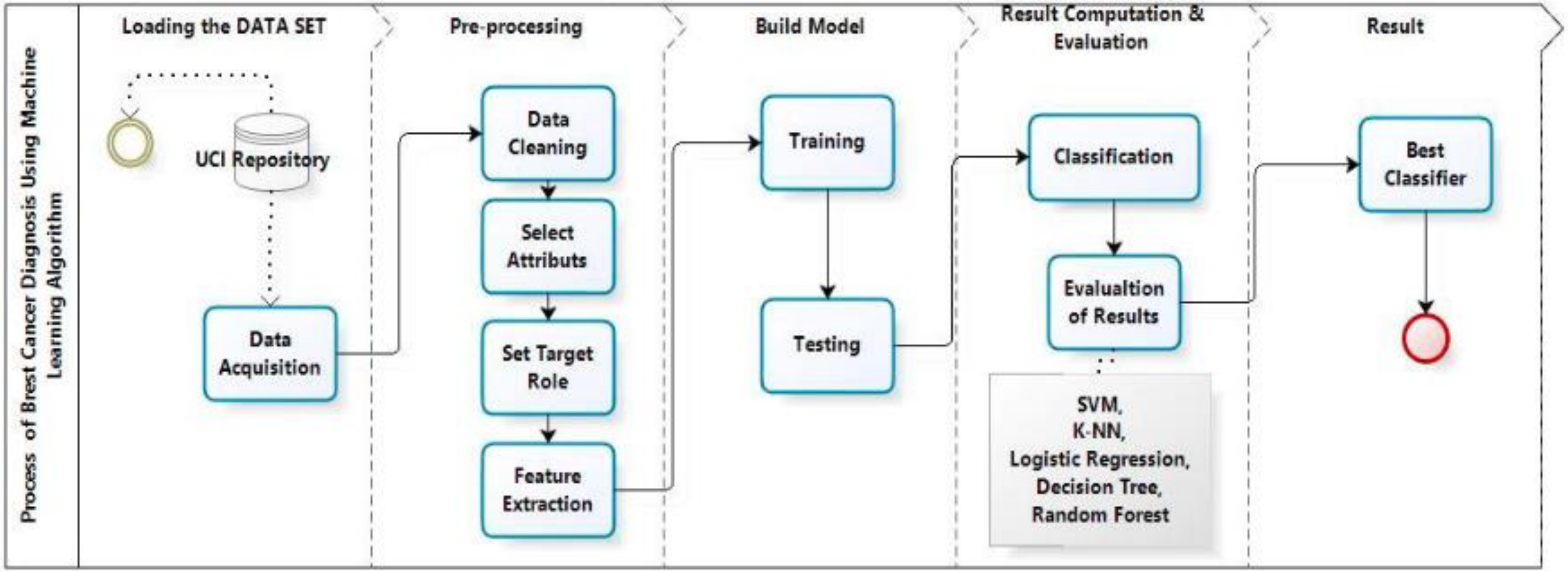
4. Methodology

Data Splitting

- **Training Set**: 60% of the data used for training the model.
- **Validation Set**: 20% of the data reserved for fine-tuning and validation of the model during training.
- **Test Set**: Remaining 20% of the data kept aside for evaluating the final performance of the trained model.

4. Methodology

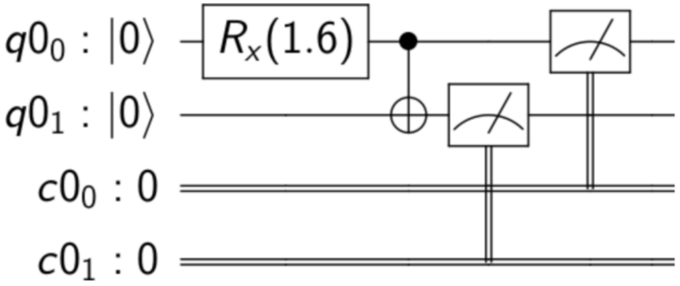
4. Classical Approach



Quantum Computing Tools - Qiskit

```
In [7]: from qiskit import QuantumRegister, ClassicalRegister, QuantumCircuit
        from qiskit.tools.visualization import circuit_drawer
        import numpy as np

        qr = QuantumRegister(2)
        cr = ClassicalRegister(2)
        qp = QuantumCircuit(qr,cr)

        qp.rx( np.pi/2,qr[0])
        qp.cx(qr[0],qr[1])

        qp.measure(qr,cr)

        circuit_drawer(qp)
```

Out[7]:



Developer(s)	IBM Research, Qiskit community
Initial release	March 7, 2017
Written in	Python
Operating system	Cross-platform
Type	SDK for Quantum Computing

4. Methodology

Qiskit

Quantum Computing Tools - Qiskit

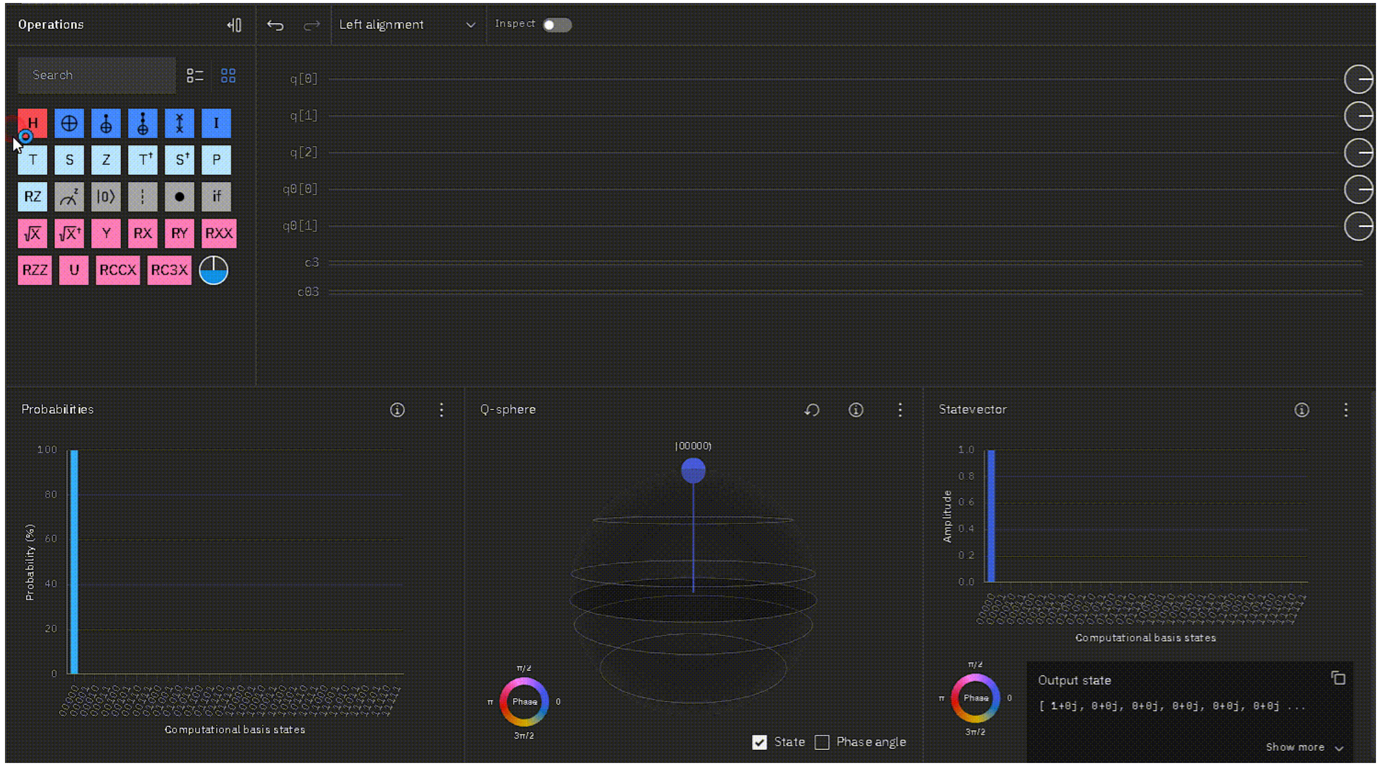
Component	Explanation
qiskit	The main Qiskit package which serves as the umbrella package that includes the core functionalities.
qiskit-aer	Provides high-performance simulators for quantum circuits.
qiskit-algorithms	Contains algorithms for quantum computing including optimization, chemistry, and machine learning algorithms.
qiskit-aqua	Provides algorithms for quantum computing applications in chemistry, AI, and optimization.
qiskit-ibmq-provider	Allows access to IBM Quantum devices and simulators.
qiskit-ignis	Provides tools for quantum error correction and mitigation.
qiskit-machine-learning	Contains quantum machine learning algorithms and tools.
qiskit-terra	Includes the necessary tools for creating and manipulating quantum circuits, compiling, and running them on quantum hardware or simulators.

```
!pip list | grep qiskit
```

```
qiskit                      0.33.1
qiskit-aer                  0.10.3
qiskit-algorithms           0.3.0
qiskit-aqua                 0.9.5
qiskit-ibmq-provider        0.18.2
qiskit-ignis                0.7.0
qiskit-machine-learning     0.3.1
qiskit-terra                0.19.1
```

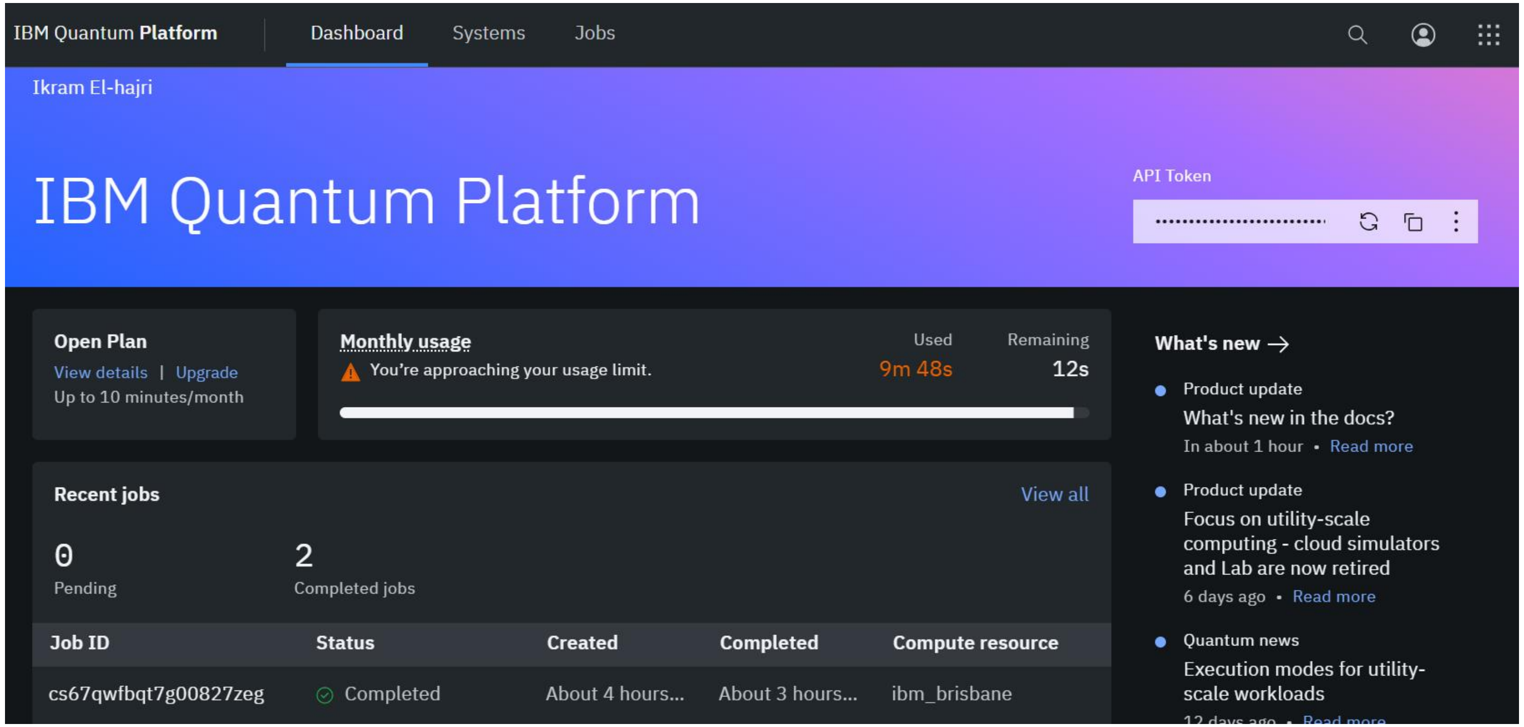
4. Methodology

Quantum Computing Tools - IBM Quantum Composer



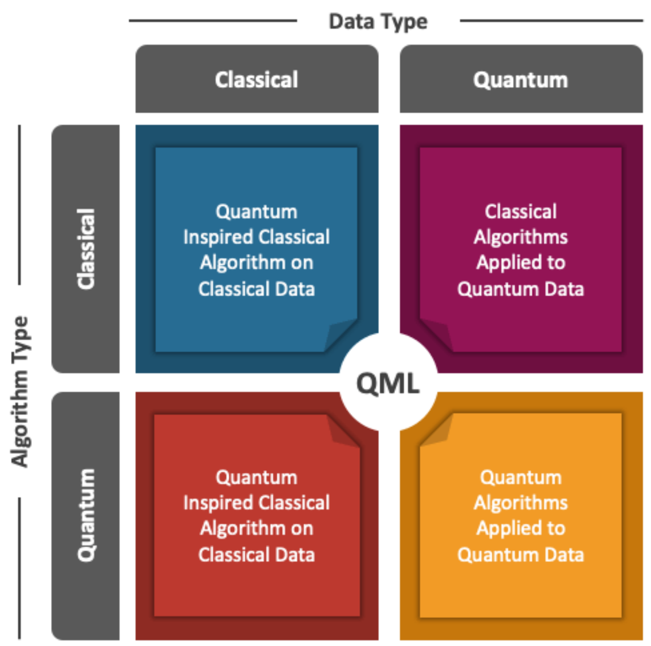
4. Methodology

Quantum Computing Tools - IBM Quantum Platform



4. Methodology

Quantum Machine Learning (QML)



CC :

- Uses traditional data treatment methods.
- Incorporates machine learning techniques inspired by quantum information research.

QC :

- Explores machine learning's role in enhancing quantum computing.
- Helps in analyzing measurement data and identifying quantum states.

CQ :

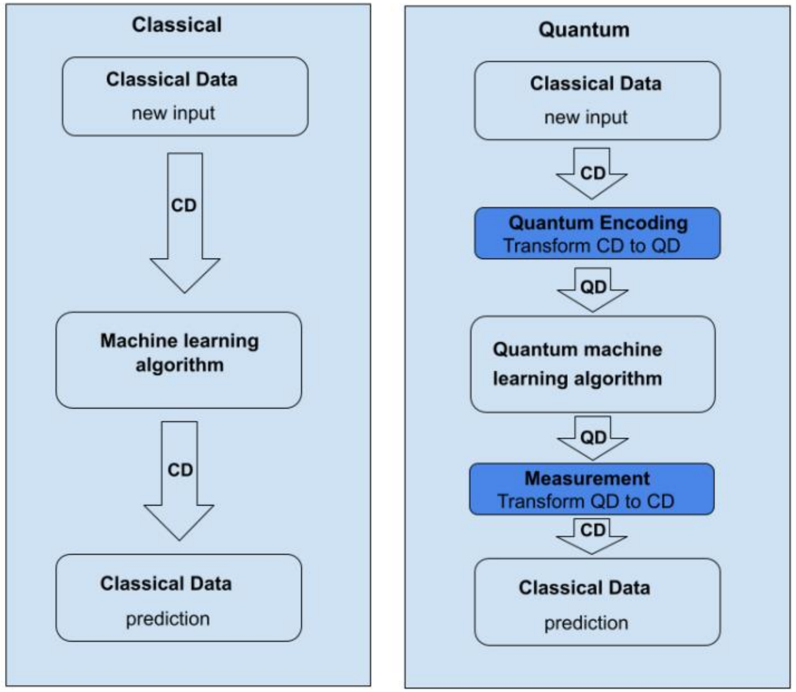
- Applies quantum computing to analyze classical datasets.
- Aims to develop quantum algorithms for data mining.

QQ:

- Focuses on processing quantum data with quantum devices.
- Analyzes experimental data or simulates behavior of quantum systems.

4. Methodology

Processing techniques of conventional machine learning and quantum machine learning.



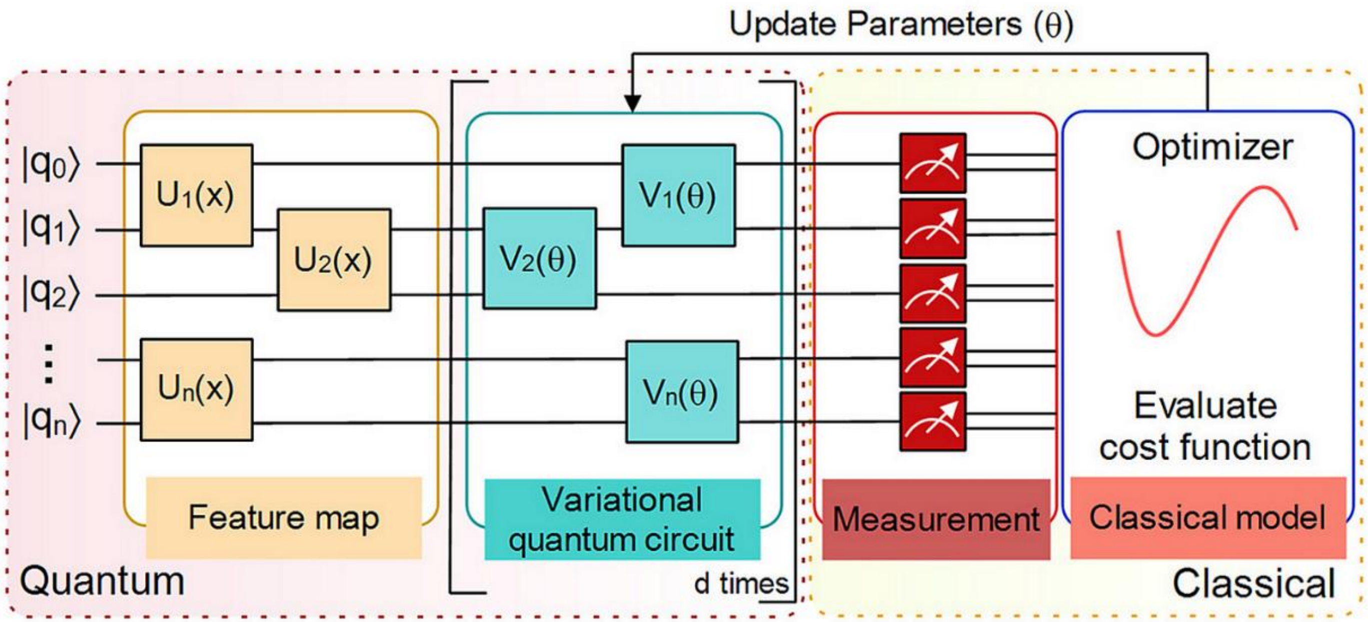
Conventional Machine Learning:

- Data is directly input to the algorithm.
- Algorithm analyzes the data and produces an output.

Quantum Machine Learning (QML):

- Requires initial encoding of data into quantum form.
- Receives quantum data as input, processes it, and generates quantum data as output.
- Quantum data is then converted back to conventional form.

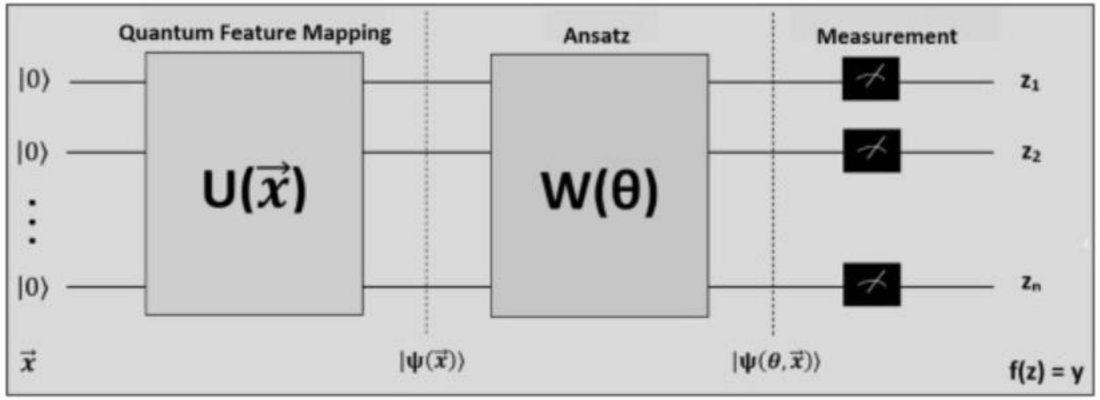
Variational Quantum Classifier (VQC)



Credit : Plos one

4. Methodology

Variational Quantum Classifier (VQC)

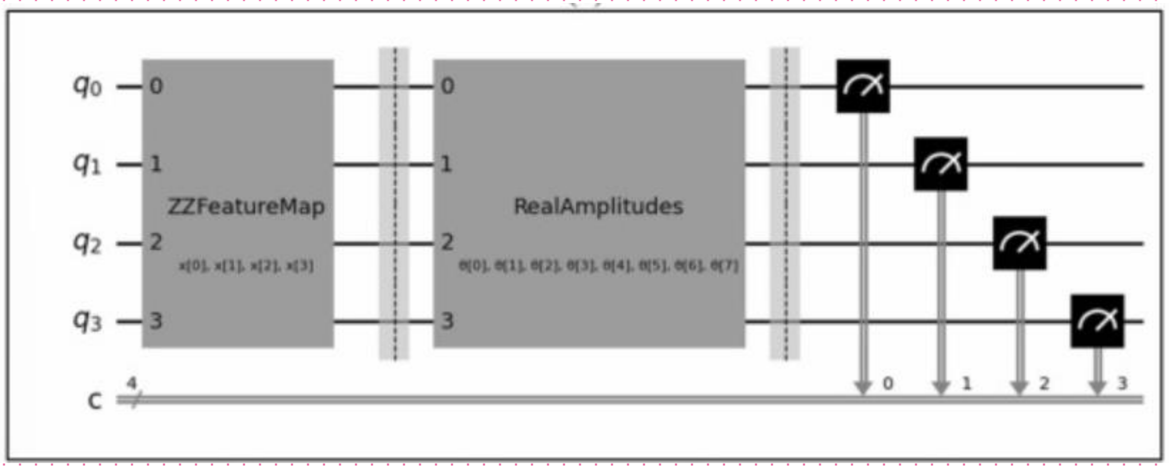


$$\mathrm{U}\left(\vec{x}\right)|0\rangle = \left|\psi\left(\vec{x}\right)\right\rangle$$

$$\left|\psi\left(\theta, \vec{x}\right)\right\rangle = \mathrm{W}(\theta)\mathrm{U}\left(\vec{x}\right)|0\rangle$$

4. Methodology

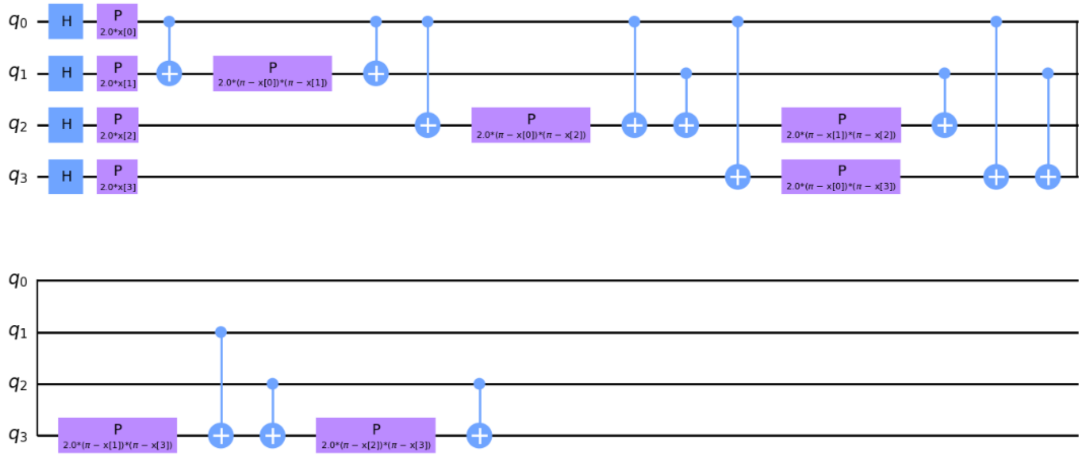
Variational Quantum Classifier (VQC)



The proposed VQC component consists of ZZFeatureMap as quantum feature mapping, RealAmplitudes as ansatz, and measurements.

4. Methodology

```python
from qiskit.circuit.library import ZZFeatureMap
feature_map = ZZFeatureMap(feature_dimension=num_features, reps=1)
```



Feature Map Encoding

- Crucial step in preparing classical data for quantum circuit processing in VQC.
- Involves mapping classical feature vectors to quantum states.
- Techniques include amplitude encoding or angle encoding.
- Transforms classical data into quantum states for quantum circuit operations.

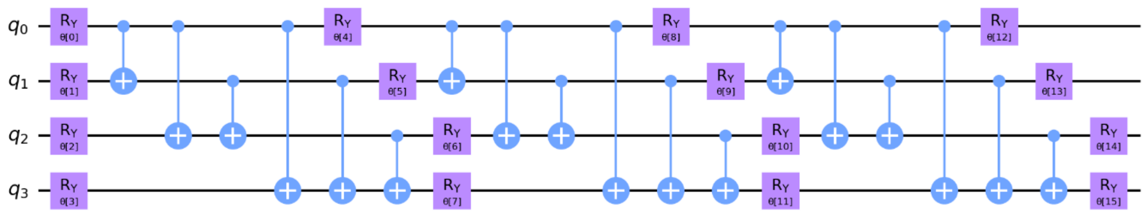
ZZFeatureMap:

- Consists of layers of Hadamard gates.
- Followed by parameterized Pauli-Z rotations.

4. Methodology

```python
from qiskit.circuit.library import RealAmplitudes
```

```python
ansatz = RealAmplitudes(num_qubits=num_features, reps=3)
```



Variational Form/ Ansatz Encoding

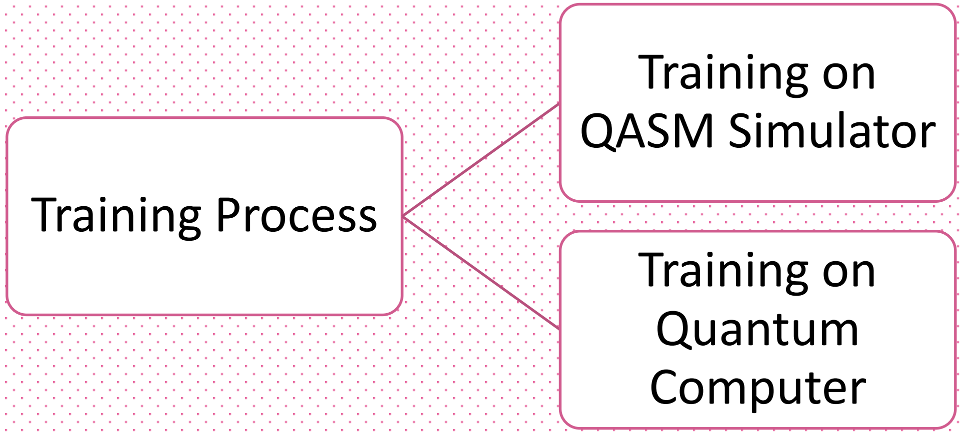
- Defines quantum circuit structure in VQC.
- Parametrized with tunable parameters.
- Parameters optimized to minimize classification errors.
- Offers flexibility for different tasks and data distributions.

RealAmplitude :

- Directly encodes real-valued amplitudes.
- Simplifies encoding, improving efficiency and accuracy.

4. Methodology

Training Approach

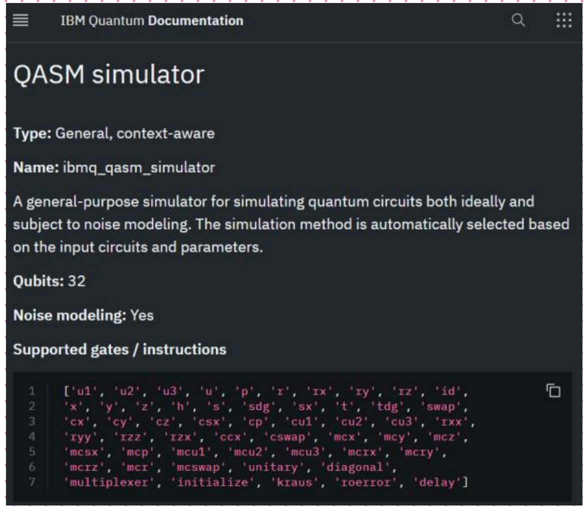


In this study, the training of the Variational Quantum Classifier (VQC) was conducted using two distinct approaches: one utilizing the QASM Simulator and the other leveraging IBM Quantum Devices.

4. Methodology

Training on QASM Simulator

```python
from qiskit import BasicAer, execute
from qiskit.algorithms.optimizers import SPSA
from qiskit_machine_learning.algorithms.classifiers import VQC
# Patch the OneHotEncoder to use sparse_output
original_init = OneHotEncoder.__init__

def patched_init(self, *args, **kwargs):
    if 'sparse' in kwargs:
        kwargs['sparse_output'] = kwargs.pop('sparse')
    original_init(self, *args, **kwargs)

OneHotEncoder.__init__ = patched_init
vqc = VQC( feature_map=feature_map,
          ansatz=ansatz,
          loss='cross_entropy',
          optimizer=SPSA(),
          initial_point=initial_point,
          quantum_instance=BasicAer.get_backend( 'qasm_simulator')
```


IBM Quantum Documentation

QASM simulator

Type: General, context-aware

Name: ibmq_qasm_simulator

A general-purpose simulator for simulating quantum circuits both ideally and subject to noise modeling. The simulation method is automatically selected based on the input circuits and parameters.

Qubits: 32

Noise modeling: Yes

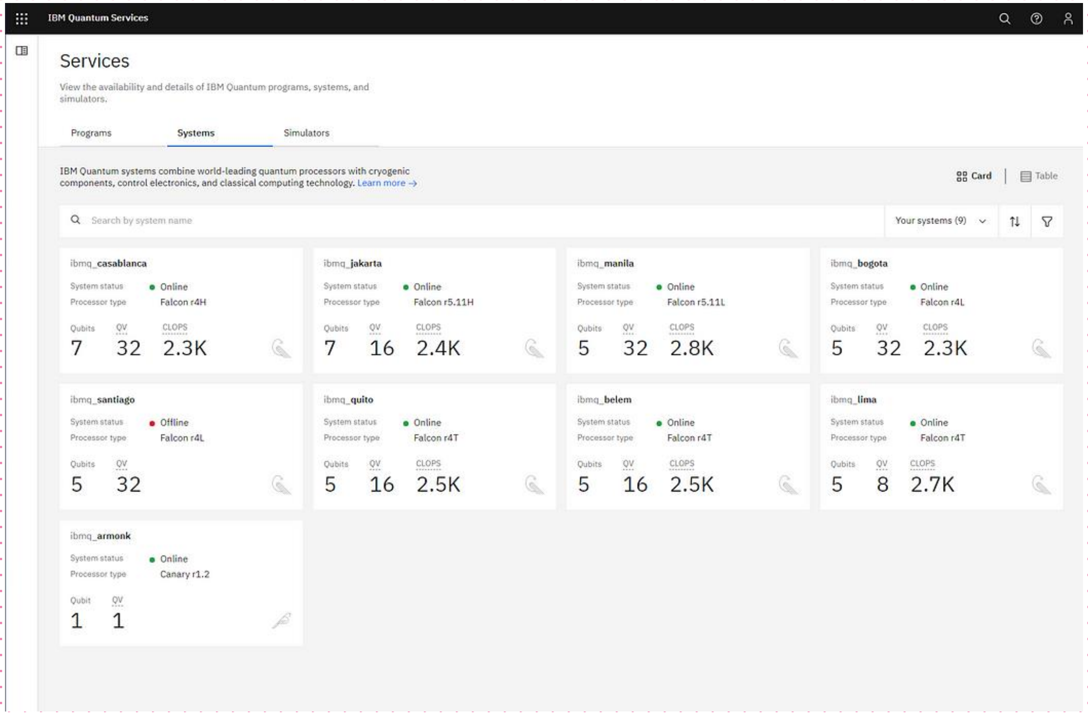
Supported gates / instructions

```
['u1', 'u2', 'u3', 'u', 'p', 'r', 'rx', 'ry', 'rz', 'id',
'x', 'y', 'z', 'h', 's', 'sdg', 'sx', 't', 'tdg', 'swap',
'cx', 'cy', 'cz', 'csx', 'cp', 'cu1', 'cu2', 'cu3', 'rxx',
'ryy', 'rzz', 'rzx', 'ccx', 'cswap', 'mcx', 'mcy', 'mcz',
'mcsx', 'mcp', 'mcu1', 'mcu2', 'mcu3', 'mcrx', 'mcry',
'mcrz', 'mcr', 'mcswap', 'unitary', 'diagonal',
'multiplexer', 'initialize', 'kraus', 'roerror', 'delay']
```

The QASM Simulator is a cloud-based quantum simulator provided by IBM Quantum, which emulates the behavior of quantum computers.

4. Methodology

```
provider = IBMQ.get_provider(hub='ibm-q', group='open', project= 'main' )
q_computer = provider.get_backend( 'ibm_brisbane')
```



Training on QASM Simulator

The second approach involved using actual IBM Quantum Devices. IBM Quantum Devices represent physical quantum processors hosted by IBM Quantum, providing access to real quantum hardware for experimentation.

4. Methodology

Optimization Process

SPSA is a gradient-free optimization technique that is particularly well-suited for optimizing black-box functions, where the gradients of the objective function are unknown or expensive to compute. It is commonly used in scenarios where traditional gradient-based optimization methods are impractical or infeasible.

Note

SPSA can be used in the presence of noise, and it is therefore indicated in situations involving measurement uncertainty on a quantum computation when finding a minimum. If you are executing a variational algorithm using a Quantum ASseMbly Language (QASM) simulator or a real device, SPSA would be the most recommended choice among the optimizers provided here.

5. Performance Comparison

5. Performance Comparison

Metrics

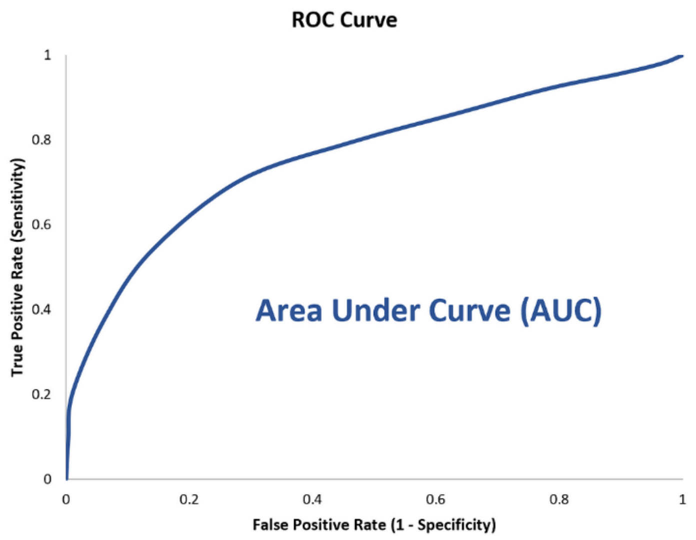
$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

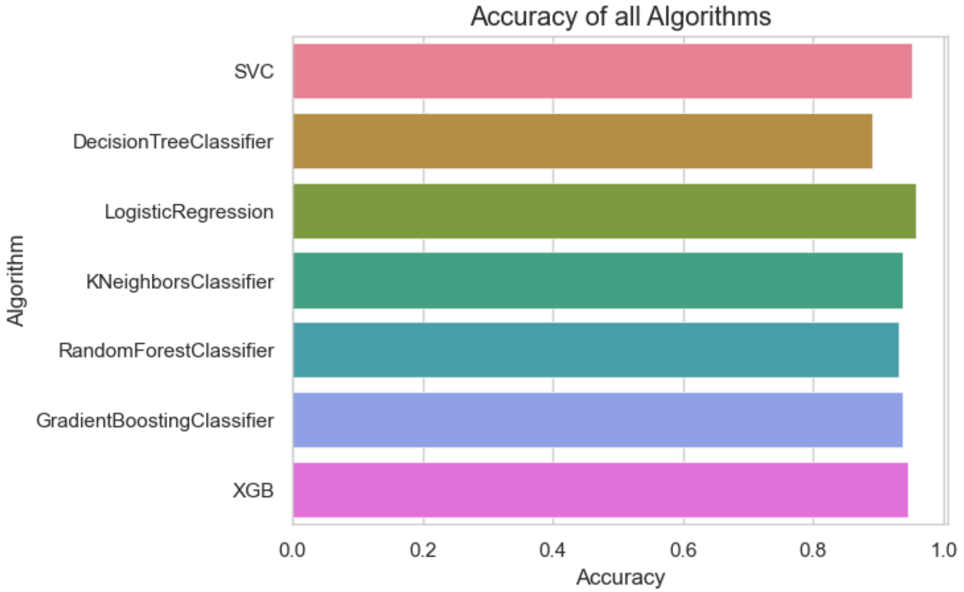
$$F_1 = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

		Predicted	
		Negative (**N**) -	Positive (**P**) +
Actual	Negative -	True Negatives (T**N**)	False Positives (F**P**) **Type I error**
	Positive +	False Negatives (F**N**) **Type II error**	True Positives (T**P**)



5. Performance Comparison

Performance of Classical Machine Learning Classifiers



Algorithm	Accuracy
SVC	**0.952055**
DecisionTreeClassifier	**0.890411**
LogisticRegression	**0.958904**
KNeighborsClassifier	**0.938356**
RandomForestClassifier	**0.931507**
GradientBoostingClassifier	**0.938356**
XGB	**0.945205**

5. Performance Comparison

	Accuracy	Precision	Recall	F1 Score	AUC-ROC score
SVM	0.95	0.90	0.97	0.93	0.97
LR	**0.96**	**0.92**	**0.97**	**0.94**	**0.98**
VQC1	0.78	0.78	0.79	0.76	0.72
VQC2	0.75	0.75	0.75	0.72	0.75

5. Performance Comparison

Time Comparison

	SVM	LR	VQC1	VQC2
Time(sec)	0.0217	0.2671	289	176297

Interpretation of Results

- VQC have significantly longer training times compared to classical models.
- Limited number of qubits and coherence times.
- Quantum Models performance can be inconsistent, with models like VQC showing significantly lower accuracy and recall.
- Quantum Algorithms are still in the experimental phase, lacking the maturity and robustness of classical algorithms.
- Quantum Computers suffer from issues like qubit decoherence, gate fidelity, and error rates.

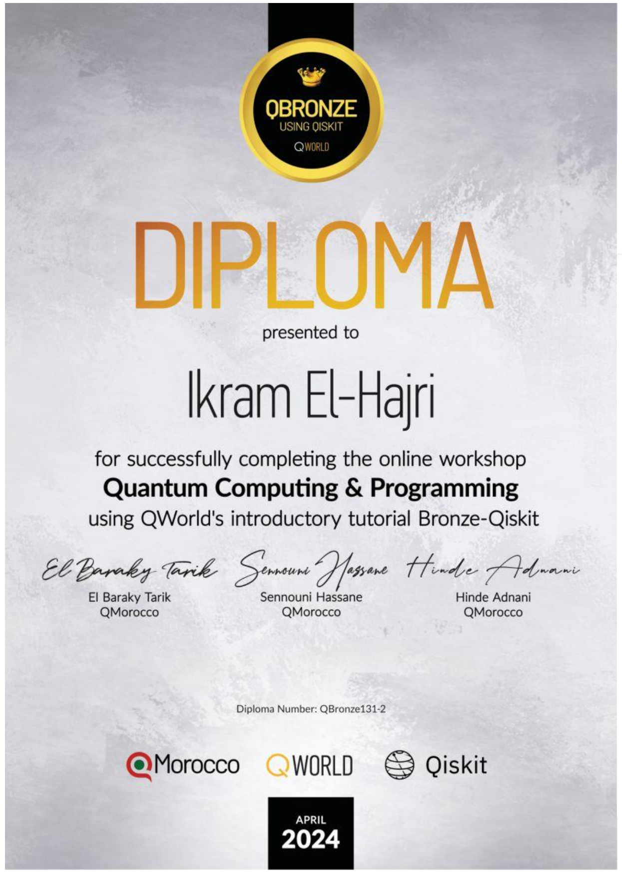
6. Conclusion & Future Directions

5. Performance Comparison

Summary of Findings

- Classical machine learning models demonstrated high accuracy in breast cancer detection, with Logistic Regression achieving the highest accuracy of 95.89%.
- Quantum hybrid models showed potential but were less consistent compared to classical methods, with performance dependent on the quality of quantum hardware and optimization techniques.

QMorocco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QMorocco
QMorocco was established in 2021 by research students and professionals. Our mission is to raise awareness about Quantum computing technology and promote it among professionals and educational institutions, and gather a community of enthusiasts in Morocco by connecting experts, educators, researchers and students in this field.
We intend to contribute to the QWorld network by organizing and participating in global programs and events, and coordinating workshops, talks and seminars. The founding members are Sennouni Hassane, a Senior Information Security Consultant, Hinde Adnani, a Ph.D student at Mohammed V University, and Zakaria Dahbi, a Ph.D student in Mathematical Physics at Mohammed V University.

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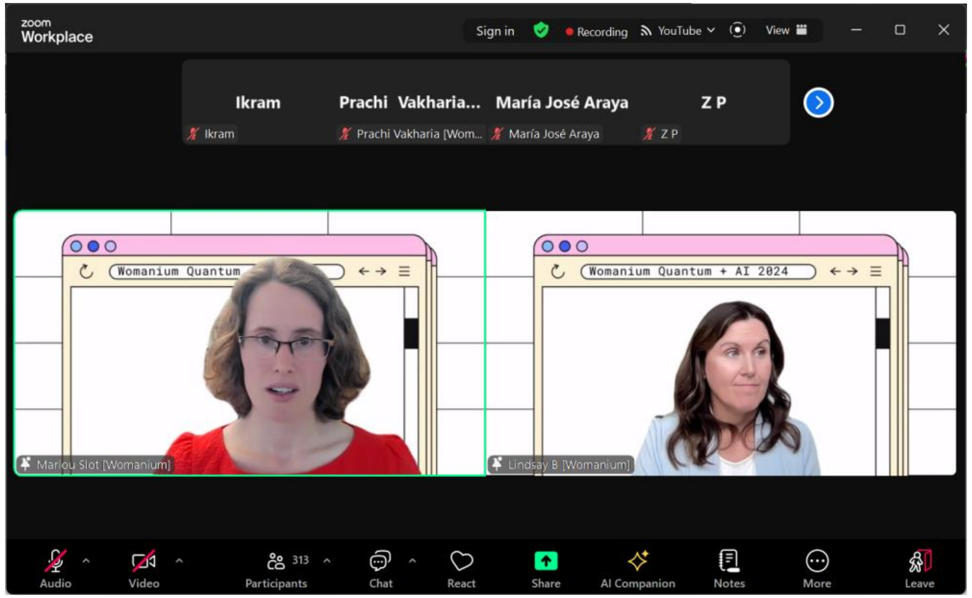

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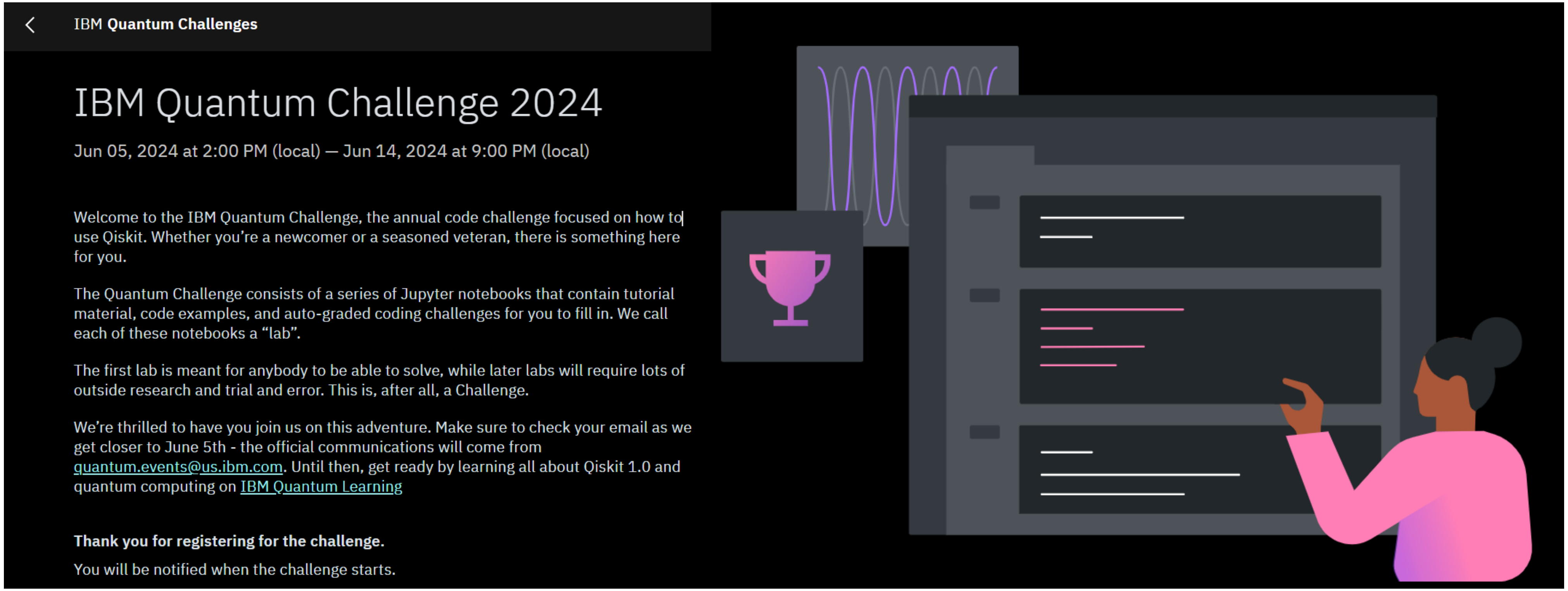

IBM Quantum Challenge 2024

Q&A

Thank You!