MODULE 7: ADVANCED ALGORITHMS AND QML OVERVIEW

CONTENTS

ADVANCED QUANTUM ALGORITHMS

Advanced Quantum Algorithms, which are designed for solving complex problems in optimization, chemistry, machine learning, and simulations. These algorithms go beyond the basics like Grover's and Shor's, and many are suitable for NISQ (Noisy Intermediate-Scale Quantum) devices.

Variational Methods:

Variational methods are mathematical techniques used to approximate solutions to complex problems—especially when an exact solution is hard or impossible to find. Main Quantum Algorithms Based on Variational Methods.

- Variational Quantum Eigensolver (VQE)
- Quantum Approximate Optimization Algorithm (QAOA)

7.1 Variational Quantum Eigensolver (VQE):

The Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical algorithm used primarily to find the **ground state energy** of a quantum system (i.e., the lowest eigenvalue of a Hamiltonian). It is one of the most practical quantum algorithms for near-term quantum computers (also known as Noisy Intermediate-Scale Quantum (NISQ) devices.

The Goal of Variational Quantum Eigensolver To solve the below equation.

$$H\,|\psi\rangle = E\,|\psi\rangle$$

Where:

- H is the Hamiltonian (energy operator) of a quantum system.
- $|\psi\rangle$ is a quantum state.
- E is the eigenvalue (energy).
- VQE aims to find the lowest energy (ground state energy) E_0 of the system.

Algorithm:

1. Ansatz (Trial State):

Create a quantum circuit with parameters θ to generate a trial wave function $|\psi(\theta)\rangle$. This is called a parameterized quantum circuit or ansatz.

2. Expectation Value Calculation (Quantum Part):

Run the circuit on a quantum computer to estimate:

$$\langle\psi(\theta) \mid H \mid \psi(\theta)\rangle$$

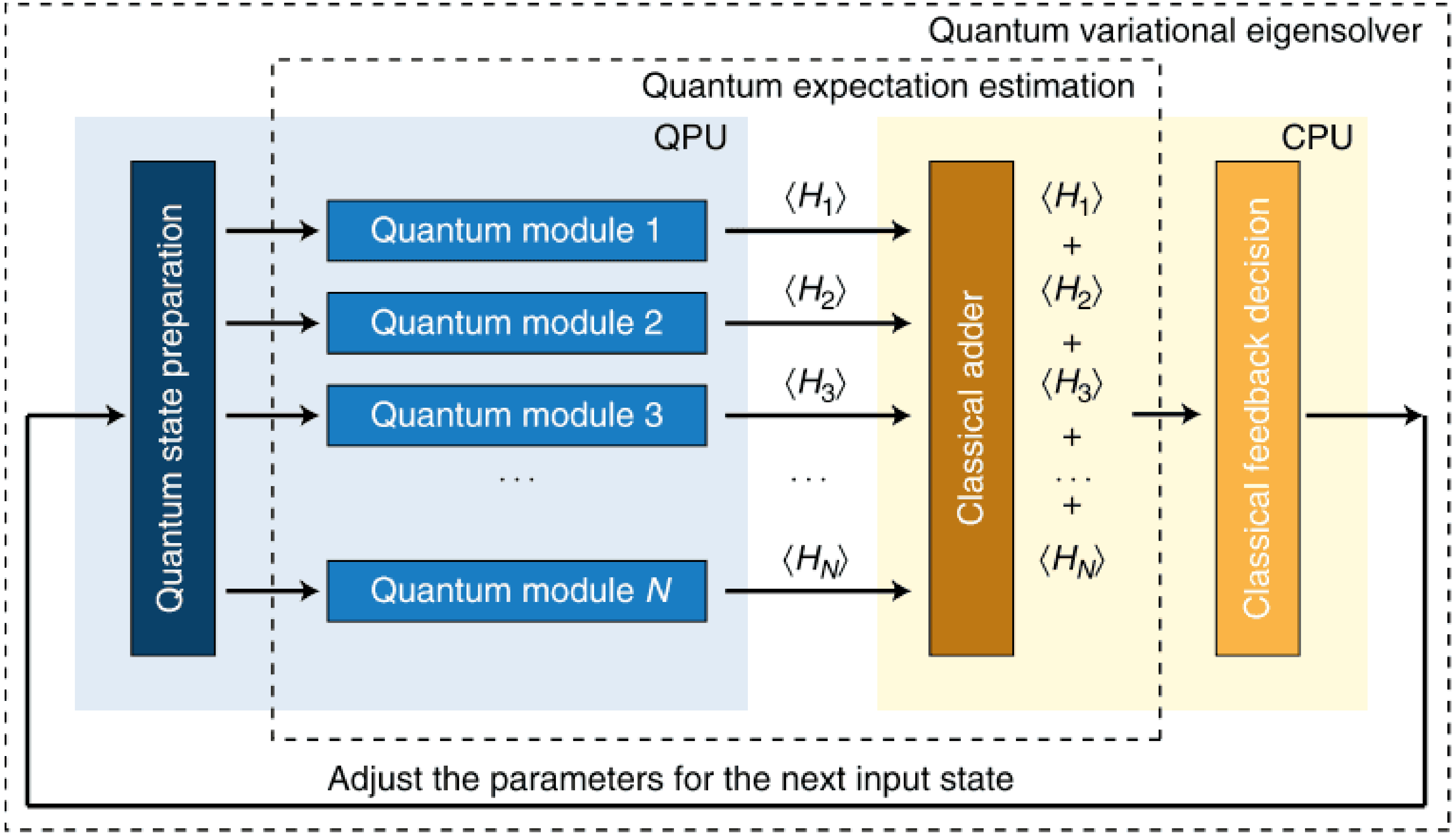
This gives an estimate of the energy for the current parameters.

3. Optimization (Classical Part):

Use a classical optimizer (like gradient descent or COBYLA) to update the parameters θ to minimize the energy.

4. Iterate:

Repeat steps 2 and 3 until convergence (lowest energy found).



Example Use Cases:

- Calculating ground state energy of molecules like H_2, LiH, or BeH_2.
- Simulating materials and quantum systems in drug discovery or materials science.

7.2 Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm (QAOA) is a hybrid quantum-classical algorithm designed to solve combinatorial optimization problems. It works by preparing a quantum state that approximates the solution to a classical optimization problem, such as Max-Cut, Traveling Salesman, or scheduling tasks.

Goal of QAOA:

To maximize a classical objective function by encoding it into a quantum cost Hamiltonian and finding a quantum state that yields the highest possible value when measured.

Find $\boldsymbol{\gamma}, \boldsymbol{\beta}$ such that $\langle \psi(\boldsymbol{\gamma}, \boldsymbol{\beta}) | H_C | \psi(\boldsymbol{\gamma}, \boldsymbol{\beta}) \rangle$ is maximized.

Where:

- H_C : Cost Hamiltonian that represents the optimization problem.

- $|\psi(\gamma,\beta)\rangle$:Quantum state prepared using alternating quantum operations.
-
- γ,β: Parameters to be optimized.

Algorithm:

1. Initial State Preparation:

Prepare a simple quantum state:

$$|s\rangle = |+\rangle^{\otimes n}$$

This is a uniform superposition over all possible solutions.

2. Construct QAOA Circuit (Ansatz):

Alternately apply two unitaries:

- **Cost unitary** based on the cost Hamiltonian:

$$U_C(\gamma) = e^{-i\gamma HC}$$

- **Mixer unitary** based on a mixing Hamiltonian H_M (usually sum of X gates).

$$U_M(\beta) = e^{-i\beta HM}$$

After p layers, the final QAOA state is:

$$|\psi(\gamma,\beta)\rangle = U_M(\beta_p)\, U_C(\gamma_p) \cdots U_M(\beta_1)\, U_C(\gamma_1)\, |s\rangle$$

3. Measurement (Quantum Part):

Measure the final quantum state and calculate the expected value of the cost function.

4. Optimization (Classical Part):

Use a classical optimizer to tune γ,β to maximize the cost function value.

5. Iterate:

Repeat the quantum-classical loop until the best parameters are found.

Example Use Cases:

Max-Cut Problem: Divide a graph's nodes into two groups to maximize the number of edges between them.

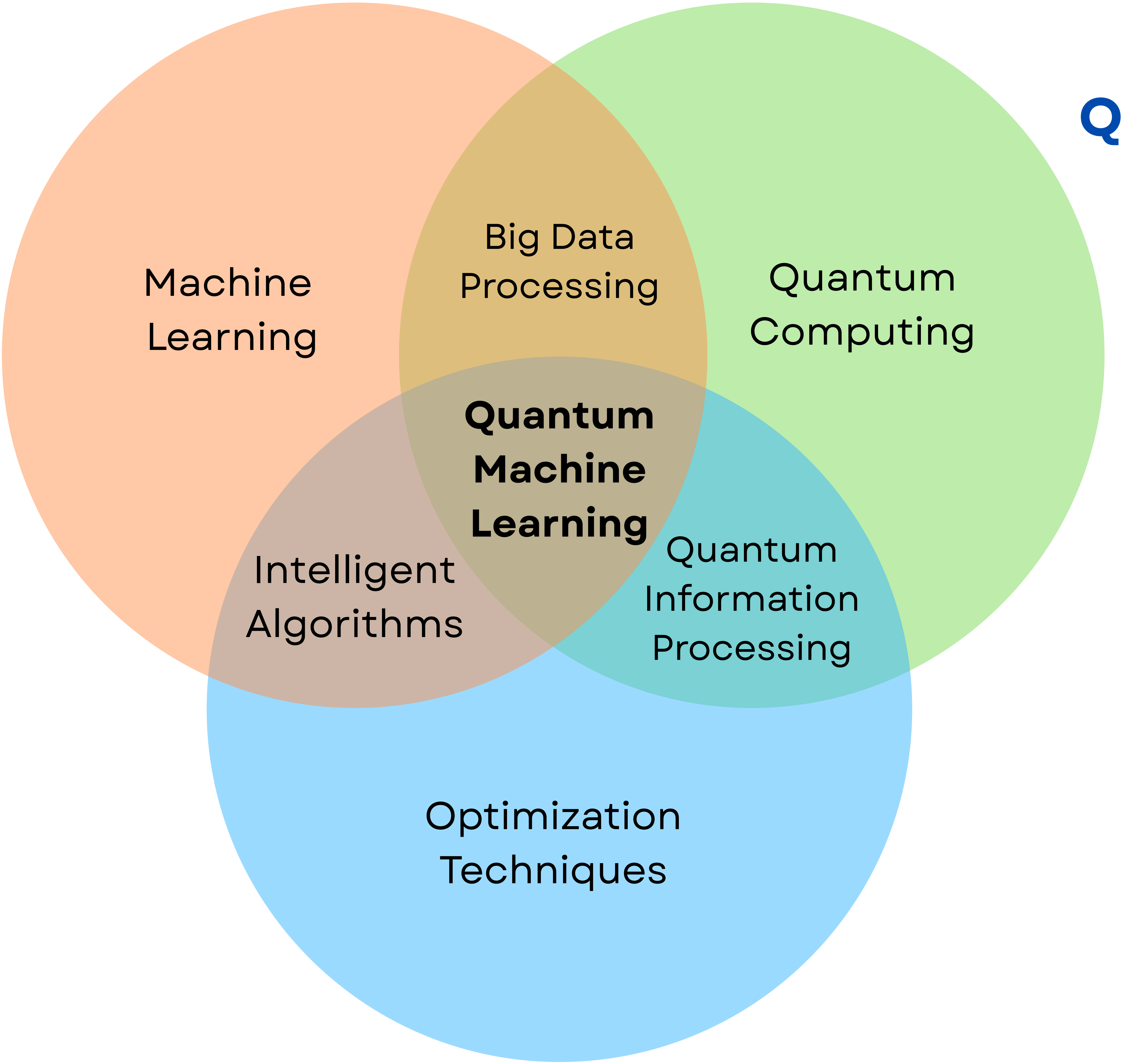
Traveling Salesman Problem (TSP): Find the shortest route visiting all cities once.

7.3 INTRODUCTION TO QUANTUM MACHINE LEARNING(QML)

Quantum Machine Learning (QML) is an interdisciplinary field that combines the principles of quantum computing with machine learning (ML) techniques to develop faster and more efficient algorithms for data analysis, prediction, and pattern recognition.

QML aims to enhance classical ML tasks (like classification, clustering, and regression) by leveraging the unique properties of quantum mechanics, such as superposition, entanglement, and quantum parallelism.

Quantum Machine Learning



Types of QML Approaches:

- **Quantum-enhanced classical ML:** Classical machine learning algorithms are augmented with quantum subroutines (e.g., quantum linear algebra or optimization).

- **Fully quantum ML:** Entirely quantum algorithms process quantum data, often requiring fault-tolerant quantum computers not yet widely available.

- **Hybrid quantum-classical:** Combines quantum and classical systems, where quantum computers handle specific tasks (e.g., feature encoding) and classical computers manage others (e.g., training).

7.4 Quantum-Classical Hybrid Algorithms

Quantum-Classical Hybrid Algorithms combine quantum processing and classical optimization to solve complex problems efficiently. They are well-suited for today's NISQ (Noisy Intermediate-Scale Quantum) computers.

Key Components of Hybrid Algorithms:

- **Quantum Subroutines** – Quantum hardware is utilized for tasks like optimization, machine learning, and simulation, where quantum advantage can provide significant speedups.
- **Classical Processing** – Classical computers manage complex control processes, error correction, and data analysis, handling parts of the problem where quantum speedup is not needed.
- **Interfacing Mechanism** – A crucial aspect is the communication between the quantum and classical systems, ensuring a smooth exchange of information and results.

Examples of Hybrid Quantum-Classical Algorithms:

Some prominent hybrid quantum-classical algorithms include:

- **Variational Quantum Eigensolver (VQE)** – Used for quantum chemistry and material science, where the quantum processor calculates the energy levels of a molecule, and the classical computer optimizes the results.

- **Quantum Approximate Optimization Algorithm (QAOA)** – Designed for combinatorial optimization problems, with the quantum processor generating candidate solutions, and the classical computer selecting the best.

- **Quantum Machine Learning (QML) –** Hybrid algorithms are applied in machine learning models where the quantum computer handles complex feature space manipulations, and classical algorithms process and refine predictions.

7.5 Advantages & Limitations of QML

Advantages

01. Quantum Speedup

02. High-Dimensional Processing

03. Quantum Feature Extraction

04. Hybrid Flexibility

Limitations

01. Quantum Noise & Decoherence

02. Limited Qubit Count

03. Lack of Quantum Datasets

04. Complex Feature Encoding

THANK YOU