Bonus Task: Quantum Computing Simulation with IBM Quantum Experience

Title:

Simulating a Quantum Circuit for Accelerated Drug Discovery using IBM Qiskit

Objective

This task demonstrates a basic quantum computing simulation using IBM Quantum Experience via Qiskit. The circuit is designed to simulate superposition and entanglement, which form the basis of quantum machine learning (QML) models used in drug discovery.

Quantum Circuit Code (Qiskit)

```
from qiskit import QuantumCircuit, Aer, execute

from qiskit.visualization import plot_bloch_multivector, plot_histogram

from qiskit.quantum_info import Statevector

import matplotlib.pyplot as plt


# Create a 2-qubit quantum circuit

qc = QuantumCircuit(2)


# Apply Hadamard gate to qubit 0 (creates superposition)

qc.h(0)


# Apply CNOT gate (creates entanglement)

qc.cx(0, 1)
```

```
# Visualize the circuit
qc.draw('mpl')
```

Simulation and Measurement:

```
# Simulate statevector
state = Statevector.from_instruction(qc)
plot_bloch_multivector(state)

# Add measurement
qc.measure_all()

# Simulate with QASM
simulator = Aer.get_backend('qasm_simulator')
result = execute(qc, simulator, shots=1024).result()
counts = result.get_counts()
plot_histogram(counts)
plt.show()
```

AI Optimization Use Case: Drug Discovery

The Problem:

AI models in drug discovery often require massive compute power to simulate molecular interactions and optimize compound selection — tasks that grow exponentially in complexity.

How Quantum Helps:

Quantum computing can simulate molecular energy states exponentially faster using quantum superposition and entanglement, outperforming classical methods. AI tasks like feature selection in molecule datasets or energy minimization for protein folding can benefit immensely.

Example:

Quantum Support Vector Machines (QSVMs) can be used to classify molecular compounds faster and with fewer features. This boosts the efficiency of AI algorithms in early-stage drug discovery, reducing time and cost.

Conclusion

This simple 2-qubit quantum circuit demonstrates the foundation of quantum parallelism. When scaled, it has the potential to revolutionize AI-powered drug discovery, enabling faster breakthroughs in pharmaceutical research.