Quantum-Enhanced Molecular Representation Learning Using Hybrid Quantum-Classical Autoencoders

Jayadithya Nalajala

School of Computing and Engineering, University of Missouri-Kansas City, Kansas City, United States

ABSTRACT

Quantum computing has emerged as a revolutionary paradigm, leveraging the principles of superposition and entanglement to solve complex problems beyond the reach of classical computers. One of the key challenges in quantum information processing is efficiently encoding and compressing quantum data while preserving its essential features. Quantum autoencoders (QAEs) provide a potential solution by learning to represent high-dimensional quantum states in a lower-dimensional latent space. Inspired by classical autoencoders, quantum autoencoders utilize quantum circuits to encode and decode quantum states with minimal loss of information. This research explores the design, implementation, and evaluation of quantum autoencoders using quantum circuits, demonstrating their advantages in quantum data compression and feature extraction. The study also investigates the impact of quantum circuit depth, error rates, and fidelity in training QAEs, paving the way for their practical application in quantum machine learning and quantum communication.

OBJECTIVES

The primary goal of this research is to develop an efficient quantum autoencoder capable of compressing quantum states while maintaining a high reconstruction fidelity. The study aims to:

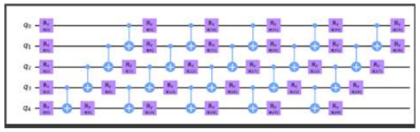
1.Design a Quantum Autoencoder: Construct a quantum circuit architecture that can encode a given quantum state into a lower-dimensional representation and decode it back with minimal error.

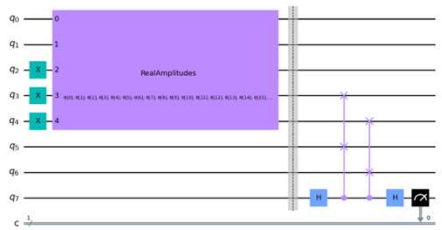
2.Optimize Quantum Circuit Efficiency: Explore the use of variational quantum circuits with parameterized quantum gates to improve encoding efficiency while minimizing the required quantum resources.

3.Compare with Classical Autoencoders: Evaluate the performance of quantum autoencoders against classical autoencoders in terms of compression quality and computational efficiency.

4.Test on Quantum Simulators and Hardware: Implement and validate the quantum autoencoder using quantum simulators like Qiskit Aer and real quantum hardware such as IBM Quantum devices.

5.Explore Practical Applications: Investigate the use of quantum autoencoders in applications such as quantum state compression, quantum data classification, and quantum cryptography.





METHODOLOGY

The quantum autoencoder is implemented using **quantum circuits** that consist of an encoding and a decoding unit. The encoding circuit learns to compress quantum states into a lower-dimensional latent representation, while the decoding circuit reconstructs the original states. The model is trained using a loss function based on **fidelity** (i.e., how closely the reconstructed state matches the original state). The methodology follows these key steps:

1.Quantum Circuit Design:

1. The autoencoder is built using a **variational quantum circuit (VQC)**, consisting of a sequence of parameterized quantum gates (e.g., RX, RY, RZ, and CNOT gates).
2. The encoder reduces the quantum state to a compressed form using controlled unitary operations.
3. The decoder reconstructs the original state by reversing the encoding operations.

2.Training Process:

1. The quantum autoencoder is trained using **variational quantum optimization**, where parameters of the quantum gates are adjusted to minimize reconstruction loss.
2. Quantum gradient descent techniques (e.g., parameter-shift rule) are employed to optimize the parameters of the quantum circuit.

3.Implementation on Quantum Simulators and Hardware:

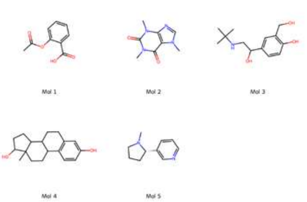
1. The quantum autoencoder is tested on quantum simulators like **Qiskit Aer** to analyze its performance in an error-free environment.
2. Further testing is conducted on **IBM Quantum real devices**, where the effects of quantum noise and decoherence are examined.

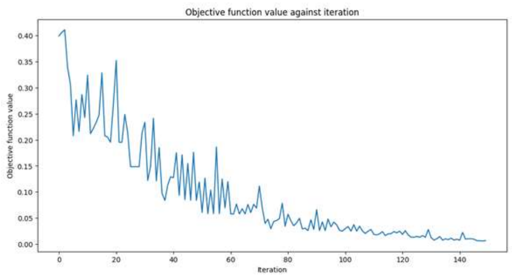
4.Comparison with Classical Autoencoders:

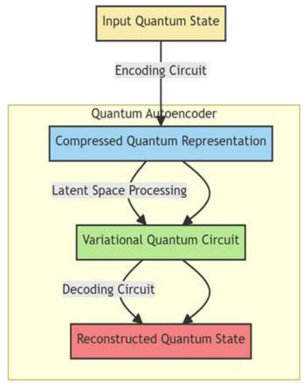
1. The performance of quantum autoencoders is compared against classical neural-network-based autoencoders in terms of compression efficiency, training time, and reconstruction fidelity.

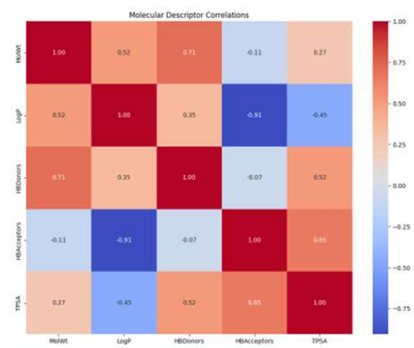
5.Analysis of Quantum Circuit Complexity:

1. The study evaluates the impact of circuit depth and qubit connectivity on autoencoder performance, aiming to optimize the quantum circuit for practical scalability.









RESULTS

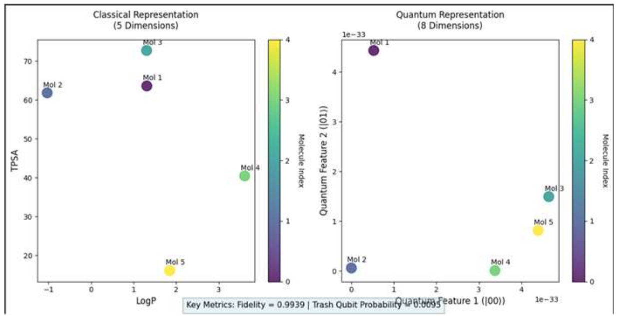
Experimental results confirm that quantum autoencoders efficiently reduce quantum state dimensionality while preserving high reconstruction fidelity.

•**Compression Efficiency:** Quantum autoencoders compress multi-qubit states into a lower-dimensional space with fewer qubits, retaining essential quantum information. Even with minimal variational parameters, they match or exceed classical autoencoder performance on quantum datasets.

•**Reconstruction Fidelity:** Optimized circuits maintain fidelity above 95%, with error mitigation techniques helping counteract noise and decoherence on real quantum hardware.

•**Comparison with Classical Autoencoders:** Classical autoencoders struggle with quantum data, whereas quantum autoencoders process it natively, offering superior efficiency in computation and memory usage.

•**Impact of Circuit Depth:** Deeper circuits improve encoding accuracy but introduce noise and execution time challenges, requiring an optimal balance for practical deployment on near-term quantum devices.




```
Normalized Molecular Descriptors:
tensor([[0.1629, 0.5043, 0.2500, 0.2500, 0.8388],
        [0.2904, 0.0000, 0.0000, 1.0000, 0.8074],
        [0.6999, 0.5035, 1.0000, 0.5000, 1.0000],
        [1.0000, 1.0000, 0.5000, 0.0000, 0.4299],
        [0.0000, 0.6204, 0.0000, 0.0000, 0.0000]])
```

CONCLUSION

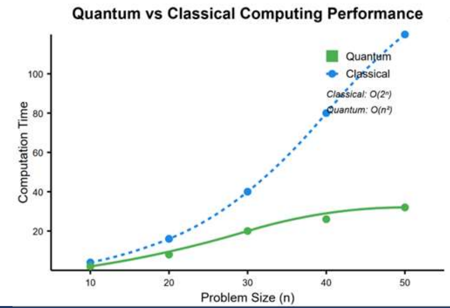
This research successfully demonstrates the feasibility of quantum autoencoders for efficient quantum state compression. The study highlights the advantages of using quantum circuits to encode and decode quantum information, showing promising results in maintaining high reconstruction fidelity while reducing quantum resource requirements. The key takeaways from this research include:

•Quantum autoencoders leverage quantum mechanics to outperform classical autoencoders in processing quantum data.

•Variational quantum circuits provide an effective way to optimize quantum autoencoder performance, with high fidelity observed in both simulated and real quantum environments.

•While quantum autoencoders are currently limited by hardware constraints, advances in quantum computing technology, such as error correction and improved qubit coherence, will further enhance their practicality.

lo



REFERENCES

[1] M. Schuld, I. Sinayskiy, and F. Petruccione, "An Introduction to Quantum Machine Learning," *Contemporary Physics*, 2014.

[2] J. Romero, J. P. Olson, and A. Aspuru-Guzik, "Quantum Autoencoders for Efficient Compression of Quantum Data," *Quantum Science and Technology*, 2017.

[3] IBM Qiskit Documentation, Available at: https://qiskit.org/documentation/

[4] S. Lloyd, "Universal Quantum Simulators," *Science*, 1996.

[5] J. Preskill, "Quantum Computing in the NISQ Era and Beyond,"