Independent Research Project Report on

Quantum State Classification Using Quantum Neural Network

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Abstract

Quantum entanglement, a nonclassical correlation between quantum subsystems, is fundamental to quantum information science and technologies like quantum teleportation, computing, and sensing. Since the Einstein-Podolsky-Rosen (EPR) paradox and Bell's inequality experiments, entanglement has challenged classical notions of locality, enabling high-dimensional entanglement in systems like photons and cold atoms.

We have used a Hybrid Quantum Neural Network (QNN) to classify quantum states as entangled or not. Datasets are simulated using Qiskit, quantum states are analyzed using features such as flattened state, purity, von Neumann entropy, fidelity, and eigenvalues of the partially transposed density matrix. A quantum circuit extracts key features, while classical neural layers refine the classification.

It was trained on a dataset of 100,000 quantum states. The hybrid model achieves high accuracy, with performance evaluated using training-validation loss trends, accuracy metrics, and a confusion matrix. This approach showcases the synergy of quantum and classical computation in solving quantum mechanics problems, advancing applications in quantum communication, error correction, and algorithm design.

Acknowledgment

I would like to express my heartfelt gratitude to the researchers whose papers have been invaluable to the success of my research. Their insightful work and contributions have provided a solid foundation for my study. The depth of knowledge and innovative perspectives shared in their research have greatly influenced and guided my approach. I am deeply appreciative of the effort and dedication they have put into their work, and I am fortunate to have had the opportunity to build upon their findings. Thank you for your invaluable contribution to the academic community.

1 Introduction

1.1 Background Theory

Quantum computing is an emerging field that leverages the principles of quantum mechanics to solve complex computational problems more efficiently than classical computing methods.

One critical aspect of quantum mechanics is the concept of quantum states, which encapsulate the information about a quantum system. A quantum state can be represented mathematically as a vector in a Hilbert space and described in terms of its wave function or density matrix.These states exhibit unique properties such as superposition, coherence, and entanglement, which enable quantum systems to perform extraordinary computational tasks. Entanglement is a pivotal feature of quantum mechanics where the quantum states of two or more particles become interdependent, such that the state of one particle cannot be described independently of the state of the other(s). This phenomenon serves as a cornerstone for many quantum technologies, including quantum cryptography, quantum teleportation, and quantum computing. However, distinguishing between entangled and separable quantum states remains a significant challenge due to the exponential growth of the Hilbert space with the number of particles, making classical approaches computationally prohibitive. Recent advancements in quantum machine learning (QML) and hybrid quantum-classical neural networks (QNNs) offer a promising approach to address this challenge. Hybrid QNNs combine quantum computing's power to process high-dimensional quantum states with classical neural networks' ability to optimize and generalize from data. This synergy makes QNNs well-suited for tasks such as quantum state classification, which involves identifying whether a given quantum state is entangled or separable.

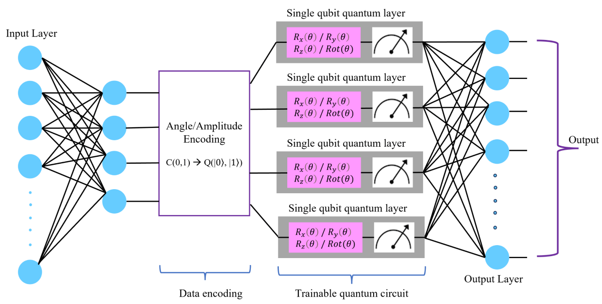

Figure 1: Hybrid QNN Architecture (Ref:Design Space Exploration of Hybrid Quantum–Classical Neural Networks by Muhammad Kashif

As quantum systems scale, the ability to efficiently classify quantum states becomes increasingly important. Entanglement detection is not only crucial for understanding the fundamental nature of quantum mechanics but also for enabling practical quantum applications such as quantum communication protocols and quantum error correction. Despite its significance, entanglement classification remains a computationally intensive task, particularly for high-dimensional or multipartite systems. Existing methods often rely on entanglement witnesses or numerical optimization techniques, which can be resource-intensive and lack scalability. The integration of hybrid QNNs offers a novel approach to tackle this issue by leveraging both quantum and classical resources. However, several challenges must be addressed to develop effective QNN models for quantum state classification. These include the design of efficient quantum circuits, the development of suitable feature encoding schemes, and the optimization of hybrid architectures to achieve high classification accuracy.

1.2 Objectives

- To study the mathematical foundations of quantum state classification.
- To design a hybrid quantum-classical neural network for quantum state classification.
- To investigate the use of QNN for classification of states.

2 Theory

2.1 Quantum Mechanics

Quantum Mechanics provides a mathematical framework to describe the behavior of particles at microscopic scales. Key principles include wave-particle duality, quantization, superposition, entanglement, and the uncertainty principle.

2.1.1 Fundamental Postulates

First Postulate: State of a Quantum System
The state of a quantum system is completely described by a wave function $|\psi\rangle$, which encapsulates all information about the system.

$$\int |\psi(r,t)|^2 \, dr = 1 \tag{1}$$

Second Postulate: Observable Postulate Every measurable physical quantity (observable) is associated with a Hermitian (self-adjoint) operator acting on the Hilbert space. For an observable represented by the operator $\hat{A}$, the eigenvalue equation is:

$$\hat{A} \, a_i = a_i \, a_i,$$

where a_i are the eigenstates and a_i are the eigenvalues (the possible measurement outcomes). Since $\hat{A}$ is Hermitian, its eigenvalues a_i are real.

Third Postulate: Measurement (Born) Postulate When a measurement corresponding to the observable $\hat{A}$ is performed on a system in state ψ, the probability of obtaining the eigenvalue a_i is given by the Born rule:

$$P(a_i) = |\langle a_i|\psi\rangle|^2 \, .$$

Immediately after the measurement—assuming an ideal measurement and a non-degenerate spectrum—the state collapses to the measured eigenstate:

$$\psi \to a_i.$$

For observables with a continuous spectrum (e.g., position), the probability density is given by:

$$P(x) = |\psi(x)|^2,$$

where $\psi(x)$ is the wave function in the position representation.

Fourth Postulate: Time Evolution Postulate The time evolution of a quantum state is governed by the Schrödinger equation. For a time-independent Hamiltonian H, the time-dependent Schrödinger equation is:

$$i\hbar \frac{\partial}{\partial t}\psi(t) = H \, \psi(t).$$

Alternatively, the state at time t can be expressed using the unitary time-evolution operator $U(t, t_0)$:

$$\psi(t) = U(t, t_0) \, \psi(t_0), \quad \text{with} \quad U(t, t_0) = e^{-iH(t-t_0)/\hbar}.$$

Since $U(t, t_0)$ is unitary, the norm of ψ remains preserved over time.

Fifth Postulate: Composite Systems Postulate For a composite system consisting of two subsystems A and B with Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, the total state space is given by the tensor product:

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B.$$

This postulate explains quantum entanglement, where a system's state cannot always be expressed as separate states of its subsystems.

Sixth Postulate: Principle of Superposition If ψ_1 and ψ_2 are valid quantum states, then any linear combination of these states is also a valid state:

$$\psi = c_1\,\psi_1 + c_2\,\psi_2,$$

where c_1 and c_2 are complex numbers. The resulting state is normalized such that

$$\langle\psi|\psi\rangle = 1.$$

3 Dataset: Tools and Features

We have generated approximately 100,000 datasets for quantum analysis.

Tools:

Qiskit:

Qiskit is an open-source quantum computing framework developed by IBM. While the current script relies on classical tools for generating random density matrices, Qiskit offers a complementary approach by enabling:

- **Quantum Circuit Design:** Creating quantum circuits to prepare specific quantum states (e.g., Bell states) in a controlled manner.
- **Simulation:** Running circuits on simulators (such as the statevector or density matrix simulators) to obtain quantum states.
- **Hardware Execution:** Executing circuits on real quantum devices available through the IBM Quantum Experience.
- **State Analysis:** Extracting quantum states from circuits and computing properties such as entanglement, fidelity, and entropy.

Integrating Qiskit into your workflow can lead to datasets generated from physically realizable quantum circuits, making the data more representative of real-world quantum experiments.

Features:

Each entry in the dataset contains several features computed from the quantum state:

1. **Flattened State:**
   The density matrix representing the quantum state is flattened into a one-dimensional list.
   Details:
   - For separable states, the density matrix is constructed as the Kronecker product of two 2×2 density matrices, resulting in a 4×4 matrix.
   - For entangled states, a 4×4 density matrix is generated directly.
2. **Entropy:**
   The Von Neumann entropy of the quantum state is computed as:

   $$S(\rho) = -\sum_i \lambda_i \ln(\lambda_i),$$

   where λ_i are the eigenvalues of the density matrix ρ.
   Purpose:
   - Measures the disorder or mixedness of the state.

- Pure states have $S(\rho) = 0$, while mixed states have higher entropy.

3. **Purity:**
   Purity quantifies how pure or mixed a state is, calculated by:

$$\text{Purity} = \text{Tr}(\rho^2).$$

   Interpretation:

   - A pure state has $\text{Tr}(\rho^2) = 1$.
   - A mixed state has $\text{Tr}(\rho^2) < 1$.

4. **Fidelity:**
   Fidelity measures the closeness of the state to the Bell state $|\Phi^+\rangle$. The Bell state is given by:

$$\text{Bell state} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

   The fidelity is computed as:

$$F(\rho, \text{Bell state}) = \text{Tr}\left(\sqrt{\sqrt{\rho}\,\text{Bell state}\,\sqrt{\rho}}\right).$$

   Purpose:

   - Provides a quantitative measure of how "Bell-like" the state is.
   - High fidelity indicates a state that is close to the maximally entangled Bell state.

5. **Partial Transpose Eigenvalues:**
   These are the eigenvalues of the density matrix after applying a partial transposition (swapping indices corresponding to one subsystem).
   Details:

   - Partial transposition is used as part of the Peres-Horodecki (PPT) criterion for detecting entanglement.
   - The presence of any negative eigenvalue in the partially transposed matrix indicates that the state is entangled.

6. **Label:**
   A binary indicator where:

   - 0 represents a separable state.
   - 1 represents an entangled state.

4 Result:

The hybrid quantum-classical neural network (QNN) was trained and evaluated for binary classification of quantum states, distinguishing between separable and entangled states.The model achieved a training accuracy of 80.7% and a test accuracy of 80.7%.

4.1 Training and Validation

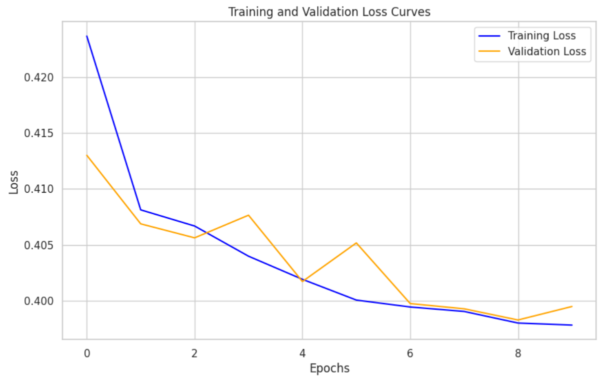

Figure 2: Training and Validation loss

The training and validation loss curves show a steady decrease over time, indicating that the model is learning effectively. The training loss is consistently lower than the validation loss, which is expected, but the gap between them remains small, suggesting minimal overfitting. Around epoch 6, both losses stabilize, showing that the model has nearly converged. The slight fluctuations in validation loss indicate some variability in unseen data but do not suggest major instability. Overall, the model generalizes well

4.2 Confusion Matrix

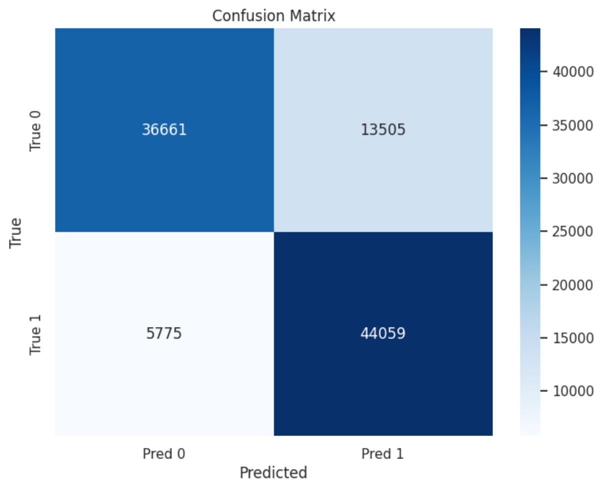

Figure 3: Confusion Matrix

A confusion matrix (Figure Y) was generated to assess classification performance in greater detail. The results indicate: True Negatives (Separable correctly classified as separable): 36,661 False Positives (Separable misclassified as entangled): 13,505 False Negatives (Entangled misclassified as separable): 5,775 True Positives (Entangled correctly classified as entangled): 44,059 These results suggest that while the model effectively identifies entangled states, it exhibits a moderate false positive rate, occasionally misclassifying separable states as entangled.

5 Discussion

In this study, we explored the use of a hybrid quantum-classical neural network to classify quantum states as either separable (labeled as 0) or entangled (labeled as 1). The model achieved a training accuracy of 80.7% and a validation accuracy of 80.7%, indicating that it was able to learn useful representations of the data while maintaining consistent performance on unseen examples.

One encouraging aspect of these results is the close alignment between training and validation accuracies. This suggests that the model is not overfitting the training data and has a good potential to generalize to new quantum states. The confusion matrix provided further insights: while the model accurately identified a large number of entangled states, there was a notable number of separable states incorrectly classified as entangled. This discrepancy points to an area where the model's discriminative power could be improved.

6 Conclusion

This study demonstrated the effectiveness of a hybrid quantum-classical neural network for classifying quantum states as separable or entangled, achieving 80.7% training accuracy and 80.7% validation accuracy. While the model performed well overall, misclassifications of separable states suggest areas for improvement, such as refining quantum feature encoding and exploring alternative circuit designs. Future work should focus on optimizing the quantum circuit, tuning hyperparameters, and comparing hybrid models to classical methods. Overall, the results show promise for using hybrid quantum-classical models in quantum state classification and further advancements in quantum information.

7 References

- Helstrom, C. W. (1969). "Quantum detection and estimation theory." *Journal of Statistical Physics, 1(2), 231–252.*
- Holevo, A. S. (1973). "Bounds for the quantity of information transmitted by a quantum communication channel." *Problems of Information Transmission, 9(3), 177–183.*
- Horodecki, R., Horodecki, P., Horodecki, M., Horodecki, K. (2009). "Quantum entanglement." *Reviews of Modern Physics, 81(2), 865–942.*
- Biamonte, J., Wittek, P., Pancotti, N., Rebentrost, P., Wiebe, N., Lloyd, S. (2017). "Quantum machine learning." *Nature, 549(7671), 195–202.*
- Farhi, E., Neven, H. (2018). "Classification with quantum neural networks on near-term processors." *arXiv preprint arXiv:1802.06002.*