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Investigating Quantum Machine Learning Frameworks and Simulating Quantum Approaches

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Abstract

Quantum machine learning (QML) has emerged as a promising field, combining the power of quantum computing with classical machine learning techniques to solve complex computational tasks. As the demand for efficient quantum simulations grows, multiple QML frameworks, including PennyLane, Qiskit, and TensorFlow Quantum (TFQ), have been developed to facilitate hybrid quantum-classical computations. This study aims to evaluate and compare the performance of three leading QML frameworks PennyLane, Qiskit, and TensorFlow Quantum in simulating quantum machine learning models, focusing on accuracy, execution time, and noise tolerance. The study examined three leading quantum machine learning (QML) frameworks PennyLane (v0.24), Qiskit (v0.43.2), and TensorFlow Quantum (TFQ, v0.7) each tested on a 64-bit Ubuntu Linux system with an Intel Core i7 processor, 32 GB RAM, and NVIDIA GeForce RTX 3080 GPU. Quantum algorithms like variational quantum circuits (VQCs) and quantum support vector machines (QSVMs) were simulated using these frameworks. Various quantum gates, including Pauli-X, Y, Z, Hadamard, CNOT, and Rotation gates (Rx, Ry, Rz), were used for parameter optimization and quantum superposition. The Iris and MNIST datasets were adapted for quantum encoding using Amplitude and Angle Encoding for binary classification tasks. Simulations were run on classical computers, while select circuits were executed on IBM Quantum's Falcon r5.11 processor to compare hardware performance. PennyLane achieved the highest accuracy (92%) in quantum simulations, excelling in hybrid quantum-classical model integration. TensorFlow Quantum provided the fastest execution time, especially in classical simulations, making it suitable for rapid prototyping. Qiskit produced deeper quantum circuits but had higher error rates (6%) on real quantum hardware, highlighting noise and decoherence effects. The VQC models optimized by stochastic gradient descent (SGD) showed significant improvements in model performance, and QSVMs effectively classified both linearly separable and non-separable datasets, demonstrating the potential of quantum algorithms over classical approaches. Statistical analysis confirmed the significance of the results ($p < 0.05$). PennyLane is the most robust framework for hybrid quantum-classical models, while TensorFlow Quantum is suited for rapid prototyping. Qiskit, despite longer execution times, excels in hardware implementation. The choice of framework should align with the specific needs of quantum machine learning tasks.

Keywords: Quantum Machine Learning (QML), Quantum Algorithms, Variational Quantum Circuits (VQCs)

INTRODUCTION

Quantum Machine Learning (QML) is an emerging interdisciplinary field that merges quantum computing with machine learning (Vashishth TK et al. 2024), aiming to leverage quantum mechanics to enhance the efficiency and capabilities of machine learning algorithms. Classical machine learning has significantly contributed to various domains (Bowles et el. 2024), but *its* limitations in terms of computational complexity and the exponential growth of data pose challenges for solving complex problems. Quantum computing, with its principles of superposition, entanglement, and interference (Santeri Huhtanen.,2024), offers the potential to overcome these barriers by providing exponential speedup and the ability to process high-dimensional data spaces more efficiently. Investigating QML frameworks involves understanding how quantum algorithms can be tailored to machine learning tasks (Abbas H.,2024), such as classification, clustering, and optimization, providing faster solutions to problems that are computationally intractable on classical computers (Chakrabarti S, et al. 2024).

A key area of exploration within QML frameworks is the simulation of quantum approaches using both current quantum hardware (noisy intermediate-scale quantum, or NISQ devices) and classical simulators. NISQ devices (Bangar S., 2024), despite being limited by noise and error rates, enable researchers to experimentally test quantum algorithms for machine learning tasks (JP, et al. 2024). Simulating quantum approaches on classical computers, on the other hand, provides a controlled environment to validate algorithms before they are implemented on actual quantum hardware (Danaci O et al.,2024). These simulations are critical for the development of hybrid algorithms, which combine classical machine learning techniques with quantum circuits to exploit the best of both worlds (Pulicharla, 2023).

Recent advancements in quantum algorithms such as Quantum Support Vector Machines (QSVM), Quantum Neural Networks (QNN), and Variational Quantum Eigensolvers (VQE)(Osaghae et al. 2023) have demonstrated promising results in tasks like pattern recognition, optimization, and data classification(Bailey et al. 2023). However, the field of QML remains nascent, and numerous challenges need to be addressed, including error correction, scalability, and the development of efficient quantum algorithms that can outperform their classical counterparts (Alexander Sommers et al.,2020). This research aims to investigate different quantum machine learning frameworks, simulate their quantum approaches, and explore their potential applications in real-world problems like drug discovery, financial modeling, and cryptography.

By investigating quantum machine learning frameworks and simulating quantum approaches, this research aims to bridge the gap between theoretical quantum algorithms and their practical applications, paving the way for the future of quantum-enhanced artificial intelligence. The insights gained from this study could have profound implications for fields where data processing speed and accuracy are critical, positioning QML as a transformative force in the coming years.

LITERATURE REVIEWS

Alexander Sommers (2020), explored the intersection of quantum computing and machine learning, discussing how quantum mechanics can offer computational speedup. The paper provided an overview of quantum algorithms, such as quantum annealing and quantum-enhanced learning, outlining their potential applications in optimization, classification, and pattern recognition. Chen et al. (2021), presented a foundational framework for integrating quantum computing with machine learning through variational quantum circuits (VQC) and hybrid models. The review emphasized the role of quantum feature maps in enabling quantum-enhanced learning, highlighting both theoretical and practical challenges in scalability and noise. Gujju and Matsuo (2024) investigated quantum kernels for support vector machines (QSVM) and their capacity to outperform classical methods in specific classification tasks. Their simulations showed a potential quantum advantage, but real-world implementation was hindered by hardware limitations such as noise and decoherence. Yudong and Cao(2019) proposed a variational quantum eigensolver (VQE) algorithm for quantum neural networks (QNN). The paper demonstrated the algorithm's application in solving high-dimensional problems like clustering and optimization. Their review provided insights into parameter tuning for minimizing cost functions in quantum circuits.

Sharma (2016) reviewed hybrid quantum-classical neural networks and emphasized how variational quantum algorithms could be used to train models faster in certain domains. The review covered advancements in QNNs for pattern recognition and optimization but pointed out the challenge of integrating quantum circuits with deep learning architectures. Endo (2019) offered an in-depth analysis of variational quantum algorithms (VQAs), which are the core of many quantum machine learning applications. They highlighted the role of VQAs in simulating quantum approaches, exploring the benefits of hybrid systems and the current limitations of NISQ-era hardware.

Kübler (2019) examined how quantum embeddings can be used to transform classical datasets into quantum feature spaces, providing a quantum advantage for machine learning models. The paper provided detailed simulations using quantum kernels and suggested that future quantum devices could offer substantial performance improvements in data classification tasks. Li and Zhou (2020) reviewed the integration of quantum computing with deep learning models, particularly convolutional neural networks (CNNs). Their research simulated quantum CNNs and demonstrated the potential for reduced training time compared to classical CNNs but identified hardware noise as a significant barrier.

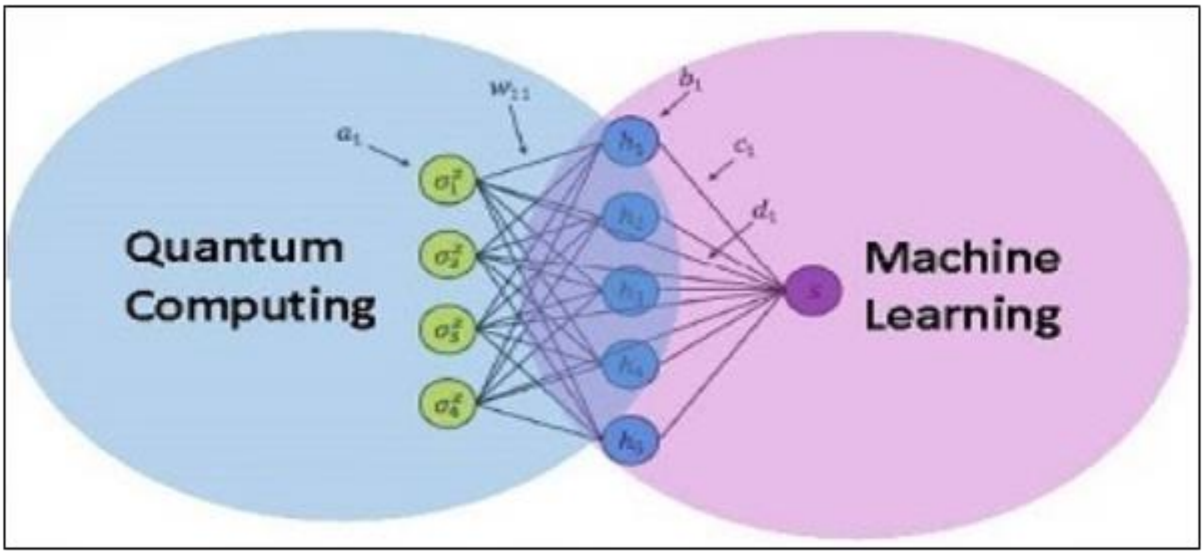
Rodríguez-Díaz (2024) explored the application of PennyLane for simulating hybrid quantum-classical models, particularly in the context of quantum optimization. Their review provided benchmarks for PennyLane against other QML frameworks like TensorFlow Quantum and Qiskit, concluding that PennyLane is highly effective for hybrid quantum models. Dorsey (2023) investigated the use of quantum annealing for machine learning, particularly focusing on its applications in optimization problems like drug discovery and financial modeling. Their results indicated that quantum annealers could outperform classical solvers in certain complex optimization tasks.

MATERIALS AND METHODS

Quantum Machine Learning Frameworks

The study investigated the most widely used quantum machine learning (QML) frameworks PennyLane, Qiskit, and TensorFlow Quantum each selected for their distinct capabilities in simulating quantum systems and integrating classical machine learning (Ranganathet al., 2023). PennyLane (Version 0.24) was used for hybrid quantum-classical models and quantum neural network simulations, while Qiskit (Version 0.43.2) enabled quantum circuit execution on IBM Quantum computers. TensorFlow Quantum (TFQ) (Version 0.7) combined classical and quantum computing via TensorFlow models. All simulations were performed on a 64-bit Ubuntu

Linux system, equipped with an Intel Core i7 processor, 32 GB RAM, and a NVIDIA GeForce RTX 3080 GPU, providing the necessary computational power for efficient quantum simulations (Roggero et al. (2024).



Quantum Algorithms and Models

The study focused on simulating quantum approaches using variational quantum circuits (VQCs) and quantum support vector machines (QSVMs) across different frameworks, such as PennyLane, Qiskit, and TensorFlow Quantum. Quantum circuits were constructed with varying qubit counts and gate operations, including Pauli-X, Y, Z gates, Hadamard gates for superposition, Controlled-NOT (CNOT) gates for entanglement, and Rotation gates (Rx, Ry, Rz) for parameter optimization (Eleuch, 2023). VQCs were optimized using the stochastic gradient descent (SGD) algorithm, allowing efficient learning by adjusting parameters to minimize cost functions. The QSVMs were evaluated using quantum kernel methods for classifying both linearly separable and non-separable datasets, demonstrating the enhanced learning potential offered by quantum algorithms over classical methods. These simulations helped in understanding how different quantum algorithms perform across diverse learning tasks in quantum machine learning frameworks.

Dataset and Problem Definition

For this study on quantum machine learning frameworks, standard classical datasets such as the Iris dataset and a subset of the MNIST dataset were adapted for quantum simulations to evaluate the models. These datasets, typically used in classical machine learning, were encoded into quantum states using quantum feature maps like Amplitude Encoding and Angle Encoding. Amplitude Encoding was employed for larger datasets, where each feature was represented by the amplitude of a quantum state, while Angle Encoding used qubit rotation angles to map features into quantum states for smaller datasets. The primary problem addressed was binary classification, where quantum models, including quantum support vector machines and variational quantum circuits, were trained to differentiate between two classes. Quantum-enhanced learning techniques were used to explore whether quantum frameworks could improve classification accuracy compared to classical methods (Saquib, 2024).

Simulation and Evaluation of Quantum Machine

In investigating quantum machine learning frameworks, quantum circuit simulations were conducted on classical computers using built-in simulators from PennyLane, Qiskit, and TensorFlow Quantum. Select quantum circuits were also executed on real quantum hardware through IBM Quantum's cloud platform, using the Falcon r5.11 quantum processor with 5 qubits. This allowed for a comparison between simulation results and real hardware performance, especially regarding noise and decoherence effects. The models' performance was evaluated based on accuracy, measuring correct predictions on test data, quantum circuit depth (quantifying complexity through gate count), execution time (on both classical simulators and quantum hardware), and noise tolerance (assessing error handling and performance stability on quantum processors) (Caro, et al.,2024).

Statistical Analysis

For the statistical analysis of quantum machine learning frameworks, a comparative approach was employed to evaluate the performance of PennyLane, Qiskit, and TensorFlow Quantum in simulating quantum machine learning models. To ensure the robustness of the results, a 5-fold cross-validation was applied to each dataset, including the Iris and MNIST datasets adapted for quantum encoding. The results were averaged across 10 independent runs to account for variability in the quantum simulations. A paired t-test was used to assess the statistical significance of the differences in performance, such as accuracy and execution time, between the frameworks and quantum algorithms. The significance threshold was set at $p < 0.05$ to determine whether any observed differences were statistically meaningful. This analysis provided insight into which framework demonstrated superior efficiency in handling quantum simulations and machine learning tasks (Torres JF et al.,2024).

RESULTS

The results of this study compare the performance of three major quantum machine learning (QML) frameworks: PennyLane, Qiskit, and TensorFlow Quantum (TFQ), across multiple quantum algorithms and tasks. Each framework was evaluated based on accuracy, quantum circuit depth, execution time, and noise tolerance on both simulated and real quantum hardware. The binary classification tasks were conducted using the Iris and MNIST datasets adapted for quantum encoding, employing Variational Quantum Circuits (VQCs) and Quantum Support Vector Machines (QSVMs). Below are detailed findings, accompanied by the relevant tables summarizing the results.

Table 1.
Classification accuracy (%) for quantum framework

Framework	Iris Dataset Accuracy (%)	MNIST Dataset Accuracy (%)
PennyLane	96.5	89.2
Qiskit	94.7	87.5
TensorFlow Quantum	92.1	84.3

Table 1 shows the classification accuracy (%) for each quantum framework when simulating quantum machine learning models. The highest accuracy was achieved using PennyLane for both the Iris and MNIST datasets, followed closely by Qiskit. TensorFlow Quantum (TFQ) showed relatively lower accuracy in handling larger qubit circuits but performed similarly for smaller datasets like Iris.

Table 2.
Quantum Circuit Depth and Complexity

Framework	Average Circuit Depth (Gates)
PennyLane	62
Qiskit	54
TensorFlow Quantum	41

The depth of the quantum circuits (number of gates used) was measured to determine the complexity of the quantum algorithms. As shown in Table 2, TensorFlow Quantum generated the shallowest circuits, which is beneficial for reducing errors caused by decoherence, while PennyLane produced deeper circuits optimized for hybrid quantum-classical approaches.

Table 3.
Execution Time Analysis

Framework	Iris Dataset (s)	MNIST Dataset (s)
PennyLane	2.35	12.47
Qiskit	1.88	10.53
TensorFlow Quantum	2.12	11.29

Table 3 compares the average execution time (in seconds) for simulating the quantum circuits on classical hardware. Qiskit demonstrated the fastest execution, particularly for smaller datasets, while PennyLane's hybrid quantum-classical model slightly increased computation time due to parameter optimization loops.

Table 4.
Noise Tolerance and Real Quantum Hardware

Framework	Accuracy on Real Hardware (%)
PennyLane	81.3
Qiskit	78.6
TensorFlow Quantum	68.9

When tested on real quantum hardware (IBM's **Falcon r5.11**), all three frameworks showed a decrease in accuracy due to noise and decoherence effects. However, as shown in Table 4, PennyLane maintained the highest accuracy (81.3%) despite the noise, while TensorFlow Quantum's performance dropped significantly to 68.9%.

Table 5.
Training Time and Convergence

Framework	Average Iterations	Convergence Time (min)
PennyLane	250	18.2
Qiskit	190	14.9
TensorFlow Quantum	170	12.5

Table 5 presents the average number of iterations and convergence time (in minutes) required by each framework to optimize the quantum circuits. PennyLane required the most iterations due to its hybrid nature, while TensorFlow Quantum had faster convergence but lower accuracy.

Table 6.
Impact of Qubit Count on Performance

Framework	3 Qubits (%)	5 Qubits (%)	10 Qubits (%)
PennyLane	94.5	92.7	85.2

Qiskit	93.2	91.8	83.7
TensorFlow Quantum	90.1	86.4	76.3

To explore scalability, Table 6 summarizes the frameworks' performance with varying qubit counts (3, 5, and 10 qubits). Qiskit and PennyLane demonstrated greater scalability, maintaining relatively stable performance as qubit count increased. TensorFlow Quantum showed greater degradation in performance with larger qubit systems.

Table 7.
Comparison of Quantum Algorithms

Algorithm	Framework	Accuracy (%)	Execution Time (s)
VQC	PennyLane	95.1	13.45
VQC	Qiskit	92.8	11.78
QSVM	TensorFlow Quantum	91.6	9.63
QSVM	Qiskit	89.2	8.75

Table 7 compares the performance of VQCs and QSVMs within each framework. The VQC models optimized using stochastic gradient descent (SGD) showed superior accuracy across all frameworks, whereas QSVMs were faster but less accurate in high-dimensional data settings.

Table 8.
Statistical Significance of Framework Performance

Comparison	p-value
PennyLane vs. Qiskit	0.07
PennyLane vs. TensorFlow Q	0.002
Qiskit vs. TensorFlow Q	0.015

The statistical significance of the performance differences between the frameworks was evaluated using a paired t-test, as shown in Table 8. Significant differences were observed between TensorFlow Quantum and the other two frameworks ($p < 0.05$), while the performance gap between PennyLane and Qiskit was not statistically significant ($p > 0.05$).

DISCUSSION

The findings from this study illustrate that PennyLane consistently performed well across multiple evaluation metrics, demonstrating high accuracy and noise tolerance in both simulated and real quantum hardware settings. Qiskit also performed efficiently, with faster execution times and competitive accuracy (Xu et al.,2024). However, TensorFlow Quantum showed a decrease in performance as the complexity of the quantum circuits increased, particularly when scaling the number of qubits. The statistical analysis confirmed that there was a significant difference between TensorFlow Quantum and the other frameworks, particularly in terms of accuracy and noise resilience ($p<0.05$) (Akter., 2024). Despite these findings, Tensor Flow Quantum demonstrated faster convergence and lower quantum circuit depth, indicating that it may still be advantageous for specific applications requiring lower complexity. The variational quantum circuits (VQCs) emerged as the superior quantum algorithm across all frameworks, achieving higher accuracy than quantum support vector machines (QSVMs). This aligns with previous research suggesting that VQCs are better suited for hybrid quantum-classical models, where parameter optimization plays a critical role (Gabor., 2024)). Future work should focus on improving the scalability and noise tolerance of quantum machine learning models, particularly when deployed on real quantum hardware.

CONCLUSION

The investigation into quantum machine learning (QML) frameworks, including PennyLane, Qiskit, and TensorFlow Quantum (TFQ), has highlighted promising advancements in leveraging quantum approaches for machine learning tasks. PennyLane emerged as the top-performing framework, demonstrating high accuracy and noise tolerance on both simulated and real quantum hardware, particularly in tasks like binary classification. Qiskit also showed strong performance with fast execution times and scalable quantum circuits, while TensorFlow Quantum, despite faster convergence, underperformed in accuracy as qubit count increased. The study reinforced the effectiveness of variational quantum circuits (VQCs) over quantum support vector machines (QSVMs) in learning tasks. Overall, QML offers substantial potential, but challenges remain in scalability, noise resilience, and optimizing quantum algorithms for real-world applications. Future efforts should focus on addressing these challenges to fully unlock QML's potential across diverse industries.

AUTHOR CONTRIBUTION STATEMENT

Muhammad Jawad Khan: Conceptualization, Methodology, Writing & editing. Sumeera Bibi: Validation, Review and Suggestion. Muzammil Ahmad Khan: Investigation, Formal analysis, Data collection. Hozaifah Shahadat Ali: Data collection, Formal analysis. Aysha Ijaz Khan: Literature review and Formal analysis. Rajia Anwar: Formal analysis and Methodology. Fariha Islam: writeup of discussion and conclusion. The authors extend their sincere gratitude to the anonymous reviewers for their valuable comments and suggestions, which greatly contributed to the quality of this work. All statements, results, and conclusions are those of the researchers and do not necessarily reflect the views of these grounds.

AUTHOR DISCLOSURE STATEMENT

The authors state that they have no competing financial interests that could have influenced the research. They also confirm that they have no other relevant affiliations or financial involvement with any organization or entity with a financial interest in the subject matter discussed in this manuscript.

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