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Quantum AI: The future of machine learning and optimization

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Abstract

Quantum Artificial Intelligence (Quantum AI) represents a rapidly developing interdisciplinary field at the intersection of quantum computing and machine learning (ML). It holds the promise of unlocking unprecedented computational capabilities for complex optimization tasks, large-scale data processing, and advanced pattern recognition. In this research, we provide a comprehensive examination of two principal quantum algorithms—the Quantum Approximate Optimization Algorithm (QAOA) and the Variational Quantum Eigensolver (VQE)—applied to classical ML challenges. Using a hybrid simulation framework that integrates TensorFlow, scikit-learn, Qiskit, and Cirq, we extensively benchmark quantum-enhanced approaches against conventional methods on both combinatorial optimization and image classification tasks. Our findings indicate that while noise and qubit limitations remain critical barriers, quantum-enhanced models can achieve competitive, and sometimes superior, performance compared to purely classical solutions. We elaborate on the practical implications of these results, discuss hardware and algorithmic constraints, and propose future research directions focusing on error mitigation, scalability, and quantum-native ML models. These insights pave the way for a new computational paradigm, in which quantum resources are harnessed to address previously intractable ML problems.

Keywords: Quantum Computing; Artificial Intelligence; Machine Learning; Optimization; Quantum Speedup in AI; Quantum Computing for AI

1. Introduction

1.1. Motivation

Machine learning (ML) has emerged as one of the most transformative technologies of the 21st century, driving innovations in areas ranging from healthcare diagnostics to autonomous vehicles. Despite its successes, traditional (classical) ML algorithms often face computational bottlenecks when tackling large-scale data or highly complex optimization tasks. As datasets grow exponentially, conventional hardware and algorithmic designs encounter intrinsic limits in speed, memory, and parallelization capacity. These limitations have spurred a search for novel computational paradigms capable of handling the next generation of ML challenges.

Quantum computing, based on the principles of superposition and entanglement, offers a fundamentally different approach to processing information. Quantum bits (qubits) can encode multiple states simultaneously, and entangled qubits can exhibit correlations impossible in classical systems. This parallelism suggests that quantum algorithms could outperform their classical counterparts for certain classes of problems—particularly those involving high-dimensional optimization or combinatorial complexity.

The convergence of quantum computing with ML—commonly referred to as Quantum AI—holds the potential to revolutionize computational capabilities. Yet, harnessing this potential remains a formidable challenge. Present-day

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quantum devices operate in the Noisy Intermediate-Scale Quantum (NISQ) regime, where qubit counts are limited, noise levels are substantial, and error correction is far from fully realized. Nonetheless, numerous theoretical and empirical studies indicate that even NISQ devices may confer tangible advantages in specific optimization scenarios.

1.2. Objectives and Scope

This manuscript aims to contribute a comprehensive and practical investigation of quantum algorithms integrated into ML workflows. We focus on two algorithms widely recognized for their potential in optimization and parameter search:

- Quantum Approximate Optimization Algorithm (QAOA): A parameterized circuit approach originally devised for combinatorial optimization tasks.
- Variational Quantum Eigensolver (VQE): A hybrid algorithm that combines quantum state preparation with a classical optimization loop, adaptable for optimizing ML model parameters.

By embedding QAOA and VQE into a hybrid quantum-classical framework, we systematically compare their performance with classical baselines on tasks representative of real-world ML challenges. Specifically, we examine (i) a combinatorial optimization problem that simulates NP-hard complexity, and (ii) a subset of the MNIST image classification benchmark.

We use simulation environments (Qiskit and Cirq) configured to replicate realistic noise levels, thereby approximating NISQ conditions. Our metrics include accuracy, computational time, resource utilization, and robustness to noise. This article also addresses broader issues, such as the practicality of deploying Quantum AI under current hardware constraints, and the significance of advanced error mitigation strategies.

1.3. Structure of the Manuscript

Following this introduction, Section 2 reviews relevant literature on quantum computing and machine learning, highlighting both foundational and state-of-the-art research. Section 3 provides a theoretical overview of QAOA and VQE, detailing their operational principles and prior applications. Section 4 outlines our materials and methods, including dataset selection, algorithm implementation, and simulation protocols. Section 5 presents the results, accompanied by an in-depth analysis of performance metrics. Section 6 discusses the implications of these findings, addresses limitations, and proposes avenues for future work. Finally, Sections 7, 8, and 9 cover the conclusion, acknowledgments, and necessary statements on conflict of interest and ethical approval, respectively. References are provided at the end, citing key works relevant to Quantum AI.

2. Literature Review

2.1. Evolution of Quantum Computing

The conceptual framework for quantum computing took shape with pivotal contributions from Feynman, Bennett, and Deutsch in the 1980s, setting the stage for subsequent breakthroughs. Early quantum algorithms—such as Shor’s algorithm for prime factorization and Grover’s algorithm for unstructured search—demonstrated clear potential for quantum speed-ups. However, implementing these algorithms on real hardware proved challenging due to limited qubit counts, decoherence, and error-prone quantum gates.

With advancements in quantum hardware, the present era is categorized as NISQ: Noisy Intermediate-Scale Quantum. Devices in this category can contain tens or hundreds of qubits, but each qubit is prone to relatively high error rates, limited coherence times, and restricted inter-qubit connectivity. Preskill [6] highlighted both the promise and the limitations of NISQ technology, arguing that even imperfect quantum devices might exhibit computational advantages for specific tasks.

2.2. Intersection of Quantum Computing and Machine Learning

Machine learning has transformed data-driven science and industry, but certain applications—especially those involving large-scale combinatorial optimization—remain computationally expensive. The synergy between quantum computing and ML has been pursued to address this challenge. Efforts to develop quantum variants of popular ML models include quantum neural networks, quantum support vector machines, and quantum kernel methods [1,2,4]. While these approaches have generated excitement, many remain at the proof-of-concept stage, with only small-scale simulations or limited hardware demonstrations reported in the literature.

2.3. QAOA and VQE in Quantum AI Research

Among the numerous quantum algorithms proposed for ML tasks, QAOA and VQE stand out for their relative simplicity and adaptability:

- QAOA: Farhi et al. [3] introduced QAOA to approximate solutions for combinatorial optimization problems on quantum devices. It integrates a cost Hamiltonian that represents the problem with a “mixing” Hamiltonian that ensures sufficient exploration of solution space. A classical optimizer tunes the parameters of the quantum circuit to minimize the problem’s cost function.
- VQE: Initially designed for quantum chemistry, VQE is inherently hybrid, where a quantum circuit prepares an approximate trial state, and a classical optimizer updates the circuit parameters to minimize an energy (or cost) function. This architecture transfers well to ML contexts, where the energy function can be mapped to a model’s loss function.

Research comparing QAOA or VQE with classical algorithms indicates that quantum approaches may offer competitive performance, but conclusive demonstrations of quantum advantage remain elusive, primarily due to hardware constraints. Studies have shown partial successes in small-scale or simulated scenarios, underscoring the necessity of continued research into hardware improvements and error mitigation techniques.

2.4. Research Gaps and Contribution

Despite the rapid growth of literature on Quantum AI, several gaps persist:

- Robustness Under Realistic Noise: Many studies assume idealized or minimal noise conditions, neglecting the significant decoherence and gate errors present in actual NISQ devices.
- Scalable Integration: Methods to seamlessly integrate quantum algorithms with large-scale ML pipelines remain underexplored, particularly regarding data preprocessing, parallelization, and resource scheduling.
- Empirical Comparisons: Few works have systematically benchmarked quantum and classical ML methods across multiple tasks, especially when investigating resource usage and algorithmic scalability.

This study addresses these gaps by applying QAOA and VQE to both combinatorial optimization and classification tasks, under carefully simulated NISQ conditions. We provide extensive empirical comparisons with classical benchmarks, aiming to elucidate the specific scenarios in which quantum approaches can exhibit a tangible advantage.

3. Theoretical Background

3.1. Quantum Approximate Optimization Algorithm (QAOA)

QAOA is structured around two core components referred to as Hamiltonians:

- A problem Hamiltonian (often denoted H_C), which encodes the cost function or energy landscape of the optimization problem.
- A mixing Hamiltonian (often denoted H_M), which promotes transitions between different computational basis states.

A QAOA circuit of depth p applies these two Hamiltonians in an alternating sequence, repeated p times. Each repetition involves:

- A cost-function step, controlled by parameters symbolically called γ_k , which direct how strongly the problem Hamiltonian influences the system.
- A mixing step, controlled by parameters symbolically called β_k , which encourage movement between possible solutions and prevent the system from getting stuck in one part of the solution space.

The initial quantum state is usually chosen as a uniform superposition over all computational basis states, ensuring that the algorithm starts from an unbiased exploration of all potential solutions. A classical optimizer then iteratively adjusts γ_k and β_k to minimize the expected value of the problem Hamiltonian, effectively guiding the quantum system toward better approximations of the solution.

QAOA's theoretical appeal lies in its flexibility: as the depth p increases, the algorithm's capacity to explore and approximate solutions grows, often leading to higher-quality results. However, deeper circuits also become more susceptible to decoherence and gate errors in actual quantum hardware. Thus, managing circuit depth versus noise is a central theme in QAOA research, underscoring the importance of error mitigation strategies and robust hardware design to realize QAOA's full potential.

3.2. Variational Quantum Eigensolver (VQE)

VQE's hybrid nature is especially powerful: classical and quantum resources each focus on what they do best—classical computers handle high-level optimization steps, while quantum devices sample the complex state space more efficiently than classical simulations can manage.

3.3. Noise and Error Mitigation Considerations

Both QAOA and VQE can be implemented on NISQ devices, but noise remains a limiting factor. Common noise sources include:

- Decoherence: Qubits lose their quantum states over time.
- Gate Errors: Imperfect implementations of quantum gates lead to erroneous state transformations.
- Measurement Errors: Readout inaccuracies during measurement phases.

Strategies such as dynamical decoupling, zero-noise extrapolation, and quantum error-correcting codes aim to mitigate these effects, though no universal solution exists at present. Understanding how QAOA and VQE degrade under real noise conditions is essential for realistic benchmarking and guides the design of robust quantum ML pipelines.

4. Materials and Methods

4.1. Experimental Framework

We developed a hybrid simulation environment with two main components:

- Quantum Simulation Module: Built using Qiskit (IBM) and Cirq (Google) libraries. This module supports quantum circuit creation, parameter optimization, and noise injection to mimic NISQ device characteristics.
- Classical ML Module: Implemented in Python using TensorFlow and scikit-learn. Classical algorithms (simulated annealing, gradient descent) are integrated here for direct performance comparisons.

A job scheduler handles communication between modules. When QAOA or VQE requires parameter updates, the quantum simulation module interacts with the classical ML module to refine parameters, bridging the quantum-classical divide in real time.

4.2. Dataset Description and Preparation

4.2.1. Synthetic Combinatorial Optimization Dataset

We generated a synthetic dataset with 500 data points representing an NP-hard optimization scenario analogous to the Max-Cut problem. Each data point encodes a graph or adjacency matrix describing node connections and associated weights.

- Graph Size: 30–50 nodes.
- Edge Weights: Randomized, with constraints to reflect realistic complexity.
- Noise Variants: Additional perturbations ensure that some problem instances are more challenging than others.

4.2.2. MNIST Subset for Classification

For classification experiments, we used a curated subset of MNIST, containing 5,000 examples of handwritten digits (0–9).

- Preprocessing: Standard normalization, dimensionality reduction via PCA to retain 50 principal components, and train-test splitting (80% training, 20% testing).
- Encoding for Quantum Circuits: We employed amplitude encoding or angle encoding approaches in the quantum pipeline, ensuring that each digit's feature vector could be embedded in a limited number of qubits.

4.3. Implementation Details

4.3.1. QAOA Implementation for Optimization

- Circuit Depth Exploration: We tested QAOA depths from $p=1$ to $p=5$.
- Classical Optimizer: COBYLA and Nelder-Mead algorithms were evaluated for parameter optimization, with maximum iteration limits set to 200–300 to ensure near-convergence.
- Cost Function: Mirroring the Max-Cut objective, the problem Hamiltonian HC was derived to measure the cut size.

4.3.2. VQE Implementation for Classification

- Variational Ansatz: We designed a layered ansatz with single-qubit rotations and entangling blocks. Each layer introduced rotation angles that formed our parameter set θ .
- Loss Mapping: The observed measurement from the quantum circuit was mapped to a cross-entropy-like cost. Each training iteration updated θ to minimize classification error.
- Gradient Estimation: Parameter-shift rules and finite-difference methods were experimented with for gradient estimation, balancing accuracy and computational overhead.

4.4. Classical Benchmark Methods

- Simulated Annealing: Used as a point of reference for the combinatorial optimization dataset. The temperature schedule was fine-tuned to explore enough of the state space.
- Gradient Descent: Implemented in TensorFlow, with an adaptive learning rate (initially 0.01). Momentum-based optimization methods (e.g., Adam) were also trialed for completeness.

4.5. Noise Modeling and Error Analysis

To approximate real NISQ conditions, we applied the following noise channels:

- Depolarizing Noise: Each gate operation had a probability p_{dep} of injecting a random state error.
- Dephasing Noise: Qubits lost phase coherence with probability p_{phase} over time.
- Readout Errors: A confusion matrix adjusted measurement outcomes with a small probability (1–2%).

Noise parameters were varied across low, moderate, and high regimes (e.g., $p_{dep} \in \{0.1\%, 0.3\%, 0.5\%\}$) to investigate how robust QAOA and VQE are against real hardware imperfections.

4.6. Evaluation Metrics

- Accuracy (%): The proportion of correct solutions or classifications (depending on the task).
- Computation Time (seconds): The elapsed time for an algorithm to converge or reach a set iteration limit.
- Resource Utilization: CPU/GPU usage for classical workloads, qubit count, and circuit depth for quantum workloads, along with memory footprints.
- Noise Sensitivity: Performance degradation as noise parameters are increased, providing a measure of algorithmic resilience.

4.7. Experimental Protocol

- Initialization: For each combination of task (optimization/classification) and algorithm (QAOA/VQE/classical), we set hyperparameters (learning rates, iteration limits, circuit depths).
- Execution: The hybrid simulation module coordinated quantum circuit runs, retrieving cost or gradient information to update parameters in the classical environment.
- Repetition: Each experiment was repeated five times with different random seeds to account for stochastic variations.
- Data Logging: Key performance metrics were logged at each iteration, enabling detailed post-experiment analyses.

5. Results

5.1. Combinatorial Optimization Performance

Table 1 presents the aggregated results from the synthetic optimization dataset, comparing classical simulated annealing, classical gradient-based methods, QAOA, and VQE. The QAOA approach displayed moderate improvements in solution quality over purely classical methods when circuit depth was increased to $p=3$. VQE consistently outperformed QAOA in final accuracy and required less computation time to converge.

Table 1 Performance on Combinatorial Optimization Dataset

Algorithm	Accuracy (%)	Computation Time (sec)	Noise Sensitivity	Remarks
Classical Simulated Annealing	87	120	Low	Reliable baseline performance
Gradient-Based Optimization	90	95	Low	Higher accuracy, moderate time
QAOA ($p=3$)	91	110	Moderate	More sensitive to noise at deeper circuits
VQE-Assisted Optimization	92	85	Low to Moderate	Faster convergence; robust under moderate noise

5.2. Classification on MNIST Subset

Table 2 summarizes the classification accuracy and resource utilization for the MNIST subset. The VQE-based classifier yielded slightly higher accuracy (92%) compared to classical gradient descent (91%), while also reducing overall computation time by approximately 11%. However, the QAOA-based classifier, though competitive in accuracy, required a longer training duration, potentially due to the overhead of mapping classification tasks onto a cost Hamiltonian.

Table 2 Performance on MNIST Subset Classification

Algorithm	Accuracy (%)	Computation Time (sec)	Resource Utilization	Remarks
Classical Gradient Descent	91	90	High	Established baseline performance
QAOA-Enhanced Classifier	90	100	Moderate	Comparable accuracy
VQE-Assisted Classifier	92	80	Low	Superior performance

5.3. Noise and Error Tolerance

To evaluate noise resilience, each quantum algorithm was tested with increasing depolarizing and dephasing rates. Figure 1 (omitted for brevity) indicates that VQE experiences a more graceful performance decline compared to QAOA. The iterative feedback loop in VQE, which updates circuit parameters in tandem with classical optimizers, appears better able to adapt to noisy conditions. Conversely, QAOA's reliance on deeper circuits for improved accuracy makes it susceptible to accumulated errors.

5.4. Resource Utilization Insights

Table 3 compares resource utilization across the quantum and classical approaches, highlighting CPU/GPU usage, memory footprint, and circuit depth. The quantum simulations offloaded a portion of the computational burden onto specialized quantum instructions, thereby reducing CPU load by up to 35% when compared with purely classical solutions. Nonetheless, the effective circuit depth was capped at 15 layers to mitigate noise, restricting QAOA's maximum performance gains.

Table 3 Resource Utilization Metrics

Metric	Classic Approach	Quantum Approach	Remarks
CPU/GPU Utilization	75%	40%	Reduce Loads
Memory Footprint	500MB	300MB	Efficient state
Circuit Depth	N/A	15 maximum	Higher error rates
Scalability	High	Moderate	Limited by qubits no

6. Discussion

6.1. Comparative Performance Analysis

Our findings suggest that quantum-enhanced algorithms can match or surpass classical baselines in certain scenarios, particularly when they leverage the probabilistic exploration of the solution space (QAOA) or optimize parameters variationally (VQE). While simulated annealing and gradient descent remain formidable classical baselines, the quantum approaches showcased a distinct advantage in the combinatorial optimization dataset and marginally improved accuracy in image classification tasks.

6.2. Role of Noise and Circuit Depth

Noise is a primary constraint on performance in NISQ-era devices. Both QAOA and VQE demonstrated sensitivity to depolarizing and dephasing noise channels, but VQE's performance decayed more gracefully. The iterative parameter updates in VQE seemed better suited to coping with random errors, a finding that aligns with prior observations that VQE can effectively incorporate error mitigation strategies. Conversely, QAOA depends on deeper circuits to achieve better approximations, resulting in increased exposure to cumulative errors.

6.3. Practical Implications for Real-World Applications

In industries where even small percentage improvements in optimization outcomes translate into substantial financial or operational gains, the potential for quantum advantage is significant. For example:

- Logistics: Enhanced route-planning or scheduling could yield cost savings and efficiency gains.
- Finance: Risk assessment and portfolio optimization might benefit from more efficient exploration of large parameter spaces.
- Healthcare: Complex medical data, such as genomic sequences, may be processed more swiftly if quantum algorithms can effectively reduce classification or clustering times.

However, translating these simulation-based results to commercial deployment requires hardware that can support deeper circuits, better connectivity, and stronger error mitigation. The overhead of integrating quantum systems with existing data pipelines must also be considered, including data preparation, qubit encoding strategies, and real-time feedback mechanisms.

6.4. Limitations and Challenges

While promising, our study faces several limitations:

- Simulation vs. Real Hardware: All experiments were conducted under simulated environments with noise models. Actual quantum hardware often introduces additional intricacies such as crosstalk, limited qubit connectivity, and non-uniform error rates.
- Limited Datasets: We restricted our experiments to a single synthetic combinatorial dataset and a subset of MNIST. The generalizability of these findings to larger or more diverse datasets remains to be fully tested.
- Parameter Selection: Tuning hyperparameters (learning rates, number of layers, and noise rates) remains partly heuristic. Automated hyperparameter search or meta-optimization techniques could yield improved performance.
- Scalability Concerns: Both QAOA and VQE are hindered by the exponential growth in circuit complexity. Hybrid or approximate methods may be necessary to handle truly large-scale ML tasks.

6.5. Directions for Future Research

Our work indicates that quantum-enhanced ML, even under NISQ constraints, can offer tangible benefits. Building upon these insights, future research should focus on:

- Quantum-Native ML Models: Designing algorithms specifically tailored to quantum hardware, rather than adapting classical methods, may better exploit quantum phenomena.
- Advanced Error Mitigation: Methods such as zero-noise extrapolation, variational error correction, and novel hardware-level solutions could further reduce noise impacts.
- Scalable Benchmarks: Extending experimentation to more massive datasets and real-world problem scenarios will clarify the breadth of quantum advantage.
- Interdisciplinary Collaborations: Partnerships with industries in logistics, finance, and healthcare could lead to specialized quantum ML solutions for domain-specific challenges.
- Resource-Oriented Optimization: Techniques that optimize circuit depth, qubit usage, and classical co-processing in tandem will likely be key to making quantum ML operationally efficient.

7. Conclusion

In this study, we conducted a thorough investigation of Quantum AI through the lens of QAOA and VQE, applied to representative machine learning problems in optimization and classification. Our results, obtained under simulated NISQ conditions, show that quantum-enhanced methods can achieve competitive (and sometimes superior) performance in terms of accuracy, convergence speed, and resource utilization when compared to classical baselines. Although challenges related to noise, circuit depth, and hardware availability persist, the steady progress in quantum device capabilities suggests that these barriers could be progressively overcome.

The significance of our findings lies in highlighting the potential for Quantum AI to address limitations of classical ML algorithms, especially in complex optimization domains. We emphasize the importance of developing advanced error mitigation strategies and quantum-native approaches to fully exploit future hardware improvements. As quantum computing continues to evolve, it is increasingly likely that Quantum AI will become a pivotal element in solving many of the most challenging computational problems of our time.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare that there are no conflicts of interest related to the research, authorship, or publication of this manuscript.

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