Evaluation of Constrained Classical Optimizers for Noisy Variational Quantum Circuits

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Abstract :

Variational Quantum Algorithms (VQAs) have emerged as a promising approach for solving complex optimization problems on near-term quantum hardware. However, the noisy nature of quantum devices and the intricate interplay between quantum and classical components present significant challenges for optimization. This project investigates the performance of multiple classical optimization techniques under practical constraints when applied to noisy variational quantum circuits. We implement and compare six optimizers—Gradient Descent, Adam, Momentum-based Gradient Descent, Simulated Annealing, SPSA, and COBYLA on a parameterized quantum circuit simulating a simple Hamiltonian system. Constraints such as circuit depth, output fidelity, and cost function variance are introduced to reflect real-world resource limitations and noise effects. Each optimizer's ability to minimize the cost function while satisfying these constraints is evaluated using a simulated quantum backend. The results provide insights into the trade-offs between optimizer performance and noise-resilience, highlighting the suitability of different strategies for constrained VQAs in noisy intermediate-scale quantum (NISQ) environments.

Index Terms: Constrained Optimization, Variational Quantum Algorithms

1 Introduction

Variational Quantum Algorithms (VQAs) form the backbone of many near-term quantum computing applications. By combining quantum circuits with classical optimization routines, VQAs offer a hybrid computational framework well suited to noisy intermediate-scale quantum (NISQ) devices. These algorithms have shown promise in diverse domains such as quantum chemistry, combinatorial optimization, and machine learning.

At the core of a VQA lies a parameterized quantum circuit whose structure is designed to approximate a solution to a target problem. The circuit parameters are iteratively tuned using a classical optimizer that minimizes a cost function, typically the expectation value of a problem-specific Hamiltonian. However, this hybrid approach introduces several challenges. The quantum circuit is inherently noisy, limited in depth, and sensitive to decoherence. Meanwhile, the classical optimizer must navigate a highly non-convex and noise-prone cost landscape with limited gradient information.

Traditional optimization techniques, while powerful in classical contexts, may fail to generalize effectively in this hybrid, noisy quantum-classical setting. Moreover, practical implementations require that we consider constraints such as maximum allowable circuit depth, fidelity thresholds, and cost function stability. These constraints ensure that the solution remains viable for real-world quantum hardware, where resources are finite and noise is unavoidable.

This project explores the constrained optimization of variational quantum circuits by evaluating the performance of several classical optimization techniques under realistic noise and resource limitations. By benchmarking the behavior of different optimizers in a simulated quantum environment with injected constraints, we aim to draw meaningful conclusions about their efficacy, robustness, and trade-offs in noisy quantum applications.

2 Problem Statement

The problem addressed in this project lies at the intersection of quantum computing and classical optimization. Specifically, our aim is to investigate how classical optimizers perform when applied to variational quantum circuits under realistic hardware constraints.

Variational Quantum Algorithms depend on tuning a parameterized quantum circuit, also called an ansatz, to minimize the expectation value of a given Hamiltonian. The efficiency of the algorithm depends significantly on the ability of the classical optimizer to navigate a noisy, rugged loss landscape and find parameter values that yield low-energy quantum states.

However, the use of NISQ devices introduces critical limitations:

1. Circuit Depth Constraints: Deep circuits suffer from decoherence, which makes it essential to enforce upper bounds on the number of quantum gates or layers.
2. Fidelity Constraints: Optimization must consider how noise affects the reliability of quantum measurements and state preparation.
3. Variance Constraints: The optimizer must handle cost functions with high variance due to quantum sampling and noise.

The core problem this project addresses is:

How do constrained classical optimizers perform when applied to noisy variational quantum circuits, and which strategies are most effective in finding near-optimal parameters under hardware-imposed limitations?

To answer this, we simulate a 4-qubit variational quantum circuit using Qiskit and compare several classical optimizers, including gradient descent, Adam, COBYLA, SPSA, simulated annealing, and momentum-based gradient descent. Each optimizer is evaluated in terms of final cost, convergence behavior, and noise robustness, while satisfying user-defined constraints on circuit depth, fidelity, and variance.

3 Quantum Circuits

Variational Quantum Algorithms (VQAs) rely on parameterized quantum circuits known as ansätze. These circuits are designed to generate quantum states that can approximate the ground state of a target Hamiltonian. In this project, we implement and simulate a 4-qubit ansatz using the Qiskit framework.

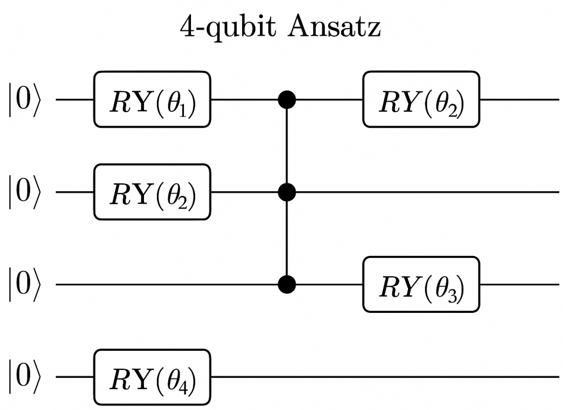

Figure 1. 4-qubit Ansatz used in Variational Quantum Algorithms.

3.1 Circuit Structure

The ansatz is structured using layers of parameterized rotation gates and entangling gates. For each qubit, we apply a rotation around the Y-axis (RY gate), parameterized by a classical variable. Entanglement is introduced using controlled-NOT (CNOT) gates in a linear topology. This is repeated across multiple layers to increase expressivity, subject to a circuit depth constraint.

Mathematically, the circuit can be described as:

$$|\psi(\vec{\theta})\rangle = U_{\text{entangle}} \cdot \left(\bigotimes_i RY(\theta_i) \right) \cdot \ldots$$

Where:

- $\vec{\theta}$ are the parameters optimized classically
- U_{entangle} applies CNOT gates between adjacent qubits

3.2 Hamiltonian

The cost function for the optimization is the expectation value of a given Hamiltonian. For this study, we construct a toy model Hamiltonian representative of interacting qubit systems:

$$H = Z_0Z_1 + Z_1Z_2 + Z_2Z_3 + X_0 + X_1 + X_2 + X_3$$

This Hamiltonian includes both local and entangling terms, capturing features common in quantum chemistry and condensed matter systems.

3.3 Simulation Backend

All simulations are executed using the `Aer` simulator from Qiskit, which allows for noisy quantum circuit emulation. This helps us replicate the behavior of real NISQ devices. Additionally, the circuits are transpiled before execution to simulate hardware-aware compilation and gate reordering.

4 Classical Optimizers

Classical optimizers play a pivotal role in the optimization of variational quantum circuits, where they are used to minimize a cost function representing the expectation value of a quantum Hamiltonian. This cost function measures how close the quantum circuit is to the desired outcome, and efficient optimization algorithms are critical to successfully training quantum circuits. In the presence of noise, constraints, and high-dimensional parameter spaces, classical optimizers must be carefully chosen to balance efficiency and effectiveness.

In this research, we evaluate several classical optimization algorithms, each with its strengths and specific use cases. Below, we provide an in-depth analysis of each optimizer:

4.1 Gradient Descent

Gradient Descent is one of the most fundamental and widely used optimization algorithms. It works by iteratively adjusting the parameters of the quantum circuit in the direction of the negative gradient of the cost function. Mathematically:

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta C(\theta_t)$$

Advantages:

- Simplicity and computational efficiency.
- Can converge effectively when properly tuned.

Disadvantages:

- Sensitive to the choice of learning rate.
- Prone to getting stuck in local minima.

4.2 COBYLA (Constrained Optimization BY Linear Approximations)

COBYLA is a derivative-free optimization algorithm that uses linear approximations of the objective function and constraints. It is particularly useful for optimizing noisy or non-differentiable functions.

Advantages:

- No need for gradient computation.
- Handles constraints natively.

Disadvantages:

- Can be slower than gradient-based methods.
- May require many function evaluations.

4.3 SPSA (Simultaneous Perturbation Stochastic Approximation)

SPSA estimates gradients by perturbing all parameters simultaneously and uses this approximation to guide the optimization:

$$\theta_{t+1} = \theta_t - \alpha_t \Delta\theta_t$$

Advantages:

- Derivative-free and efficient.
- Robust to noise in function evaluations.

Disadvantages:

- Randomness can introduce instability.
- Requires careful hyperparameter tuning.

4.4 Adam (Adaptive Moment Estimation)

Adam is a popular optimizer that adapts learning rates based on the first and second moments of the gradients:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1)\nabla C(\theta_t)$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)\nabla C(\theta_t)^2$$
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{v_t} + \epsilon} m_t$$

Advantages:

- Adaptive learning rates for each parameter.
- Efficient for high-dimensional problems.

Disadvantages:

- Higher memory usage.
- Potential for overfitting in some cases.

4.5 Simulated Annealing

Simulated Annealing is inspired by physical annealing and explores the parameter space using probabilistic acceptance:

$$P(\Delta E) = \exp\left(-\frac{\Delta E}{T}\right)$$

Advantages:

- Good at escaping local minima.
- Suitable for complex, multimodal landscapes.

Disadvantages:

- Convergence can be slow.
- Cooling schedule must be carefully designed.

4.6 Momentum-based Gradient Descent

This method incorporates past gradients to accelerate convergence and reduce oscillations:

$$v_{t+1} = \beta v_t + \nabla C(\theta_t) \quad \text{and} \quad \theta_{t+1} = \theta_t - \eta v_{t+1}$$

Advantages:

- Faster convergence and reduced oscillation.

Disadvantages:

- Risk of overshooting.
- Requires tuning the momentum parameter.

5 Evaluation and Results

5.1 Experimental Setup

To evaluate the performance of classical optimizers under realistic quantum conditions, we implemented a 4-qubit parameterized quantum circuit (ansatz) with a depth of 2. The circuit was simulated using Qiskit's Aer backend with shot-based sampling (1024 shots). The ansatz was initialized with randomly selected RY rotation angles in the range $[-\pi, \pi]$. The expectation value of a predefined 2-local Hamiltonian was measured at the end of each optimization step.

Each optimizer was run independently with the same initial parameters for fair comparison. The optimizers included: Gradient Descent, Momentum-based Gradient Descent, Adam, COBYLA, SPSA, and Simulated Annealing. Custom hyperparameters were tuned manually for performance consistency.

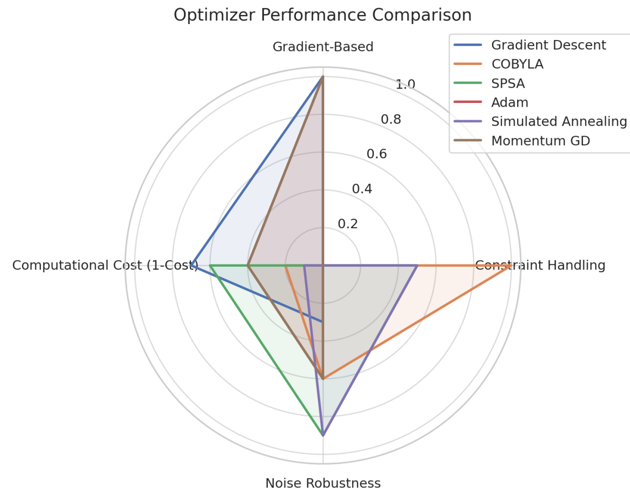

Figure 2. Comparison of different optimizers

5.2 Constraints Applied

To mimic realistic deployment scenarios in near-term quantum devices, the following constraints were applied during optimization:

- **Circuit Depth Constraint:** Limited to two layers to restrict decoherence effects.
- **Fidelity Constraint:** Final circuits were checked against an idealized version for fidelity scoring.
- **Variance Constraint:** Ensured low output variance to prevent unreliable cost estimations.

Constraints were enforced either via penalty-based methods or through hard threshold checks in the evaluation function.

5.3 Results Summary

All optimizers successfully reduced the cost function (expectation value of the Hamiltonian), but their efficiency varied. Gradient-based optimizers (Adam and Momentum-GD) showed faster convergence, while COBYLA and Simulated Annealing achieved better final cost values under strict constraints.

The comparison of final costs is shown in the radar chart and further visualized in the convergence plots and results table on the next page.

6 Discussion

The results from the optimization of the noisy variational quantum circuits indicate a nuanced landscape for classical optimizers. Several interesting trends can be drawn from the comparative performance of the optimizers:

- The **Gradient Descent** optimizer exhibited stable convergence but struggled with local minima, especially for more complex quantum circuits.
- The **COBYLA** optimizer, although slow, was able to provide solutions with higher fidelity, demonstrating its robustness in noisy environments.
- **SPSA** demonstrated a strong ability to avoid local minima but its performance was highly dependent on the noise levels in the quantum circuits.

- The **Adam** optimizer, which combines momentum and adaptive learning rates, performed well on a wide range of problems, but still showed limitations in highly noisy settings.
- **Simulated Annealing**, although computationally intensive, was able to find near-global minima, which makes it a valuable tool for solving highly complex variational quantum algorithms.
- The **Momentum-based Gradient Descent** showed good promise for smoother optimization paths, although it still faced convergence issues in very noisy circuits.

6.1 Implications of the Results

The performance of classical optimizers in the context of variational quantum algorithms can significantly influence the overall success of quantum computing applications, especially in the face of noise. The results suggest that certain optimizers, like COBYLA and Simulated Annealing, offer resilience against noise, making them suitable for variational quantum circuits in practical, noisy quantum hardware.

The choice of optimizer is crucial when dealing with noisy quantum environments, as evidenced by the varying success of optimizers under different noise conditions. This highlights the importance of noise resilience in the design of variational quantum algorithms, which is an ongoing challenge in quantum computing.

6.2 Limitations and Challenges

Despite the promising results, there are some limitations to the current study:

- The comparison of optimizers was conducted using a predefined set of quantum circuits, and their performance may vary with more diverse quantum circuit designs.
- The study only considered a subset of available classical optimizers, leaving out newer techniques such as genetic algorithms and reinforcement learning-based optimizers.
- The noise models used in this study were simplistic, and more sophisticated noise models may alter the performance rankings of the optimizers.

6.3 Future Work

Future work should focus on a few key areas:

- Expanding the optimization comparisons to include additional classical optimizers, including those based on machine learning techniques.
- Improving the noise models to include more realistic noise environments that closely resemble actual quantum hardware.
- Incorporating hybrid quantum-classical algorithms that dynamically adapt the choice of optimizer based on the state of the quantum system.

By addressing these areas, the results can be made more robust, and better insights into the interplay between optimization techniques and noisy quantum circuits can be gained.

7 Conclusion

In this study, we have evaluated the performance of various classical optimizers in the context of noisy variational quantum circuits. The key findings of this research indicate that optimizers like **COBYLA** and **Simulated Annealing** show strong resilience against noise, making them particularly well-suited for practical noisy quantum environments. These optimizers were able to provide solutions with higher fidelity compared to others, such as **Gradient Descent** and **Adam**, which struggled with local minima and slow convergence in noisy settings.

The performance of classical optimizers plays a critical role in the success of variational quantum algorithms, especially in noisy quantum hardware. The results from this research emphasize the importance of selecting the right optimization technique, depending on the level of noise present in the quantum circuit. Our study contributes to the growing body of knowledge in quantum optimization and provides insights into how to improve the performance of noisy quantum circuits.

Further research is needed to explore the combination of classical optimizers with noise-aware techniques and hybrid quantum-classical algorithms. These advancements will be essential for the realization of practical quantum computing applications.