Simulation and Noise-Aware Evaluation of Grover's Algorithm using Qiskit

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Abstract

This paper presents a rigorous simulation of Grover's algorithm on a 2-qubit system using IBM's Qiskit framework. I analyzed the algorithm's performance in both ideal and noisy quantum environments, incorporating hardware-specific noise models. The work aims to bridge the gap between theoretical quantum computing and practical NISQ-device experimentation, providing an accessible yet technically sound framework for early-stage researchers.

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1 Introduction

The pursuit of quantum advantage, solving problems intractable for classical computers, has evolved from a theoretical concept to an experimental reality. Among the most renowned quantum algorithms demonstrating computational speedup is *Grover's search algorithm*, which provides a quadratic reduction in query complexity for unstructured search problems. Although Shor's factoring algorithm often garners significant attention, Grover's algorithm is more accessible for instructional purposes and demonstrates a fundamental and generalizable quantum technique, **amplitude amplification**. Classically, searching an unsorted list of N elements requires $\mathcal{O}(N)$ queries. Grover's algorithm reduces this to $\mathcal{O}(\sqrt{N})$, representing a significant improvement in computational efficiency. While the speedup is not exponential, it is applicable to a wide range of practical tasks, including cryptographic key searching, optimization, and database querying.

Despite its theoretical appeal, the physical implementation of Grover's algorithm remains largely pedagogical, particularly in the current era of Noisy Intermediate-Scale Quantum (NISQ) devices. These systems face challenges such as limited qubit coherence, low gate fidelity, and short decoherence times. As a result, simulating quantum algorithms remains essential for understanding their behavior prior to deployment on real hardware. **Qiskit**, an open-source software development kit by IBM, offers a powerful platform for designing, simulating, and executing quantum circuits, complete with support for both ideal and noisy quantum backends.

This work presents a rigorous simulation and performance evaluation of Grover's algorithm for a 2-qubit system, implemented using Qiskit. Our objectives are twofold:

1. To demonstrate the full lifecycle of a quantum algorithm, from theoretical formulation to circuit implementation and simulation.

2. To assess the impact of realistic noise on the success probability of Grover's algorithm.

This study distinguishes itself from prior educational implementations through its adherence to gate-level details reflective of real IBM Q processors and its use of custom noise models based on actual hardware calibration data. The simplicity of a 2-qubit search space allows for exact analytical expectations while providing a concrete platform to explore fidelity loss, oracle construction, and measurement error. Our goal is to bridge the gap between introductory quantum computing and publishable scientific research. This is particularly relevant for students and early-career researchers seeking meaningful contributions without formal academic affiliation or access to laboratory infrastructure.

Moreover, the pedagogical benefits of such simulations are immense. By working with simplified yet representative models, learners can internalize critical aspects of quantum logic, such as entanglement, measurement collapse, and unitary evolution. The ability to simulate both perfect and noisy conditions enables a practical appreciation of error mitigation and the realities of hardware-level imperfections, insights often abstracted away in purely theoretical studies. The reproducibility of this framework enhances its value not only as a research prototype but also as a tool for curriculum development and laboratory instruction. Since Qiskit is accessible and extensible, this work may serve as a modular foundation for coursework in quantum programming, quantum algorithms, or quantum information theory.

While this work centers on Grover's algorithm due to its relative simplicity and broad relevance, the methodology generalizes to other algorithms such as Deutsch–Jozsa, Bernstein–Vazirani, and even variational quantum circuits. In each case, noise modeling and simulator calibration offer opportunities to assess hardware-readiness and predict execution outcomes across platforms. Lastly, we acknowledge the limitations imposed by the small system size. A 2-qubit database search represents the most basic non-trivial Grover implementation, insufficient for demonstrating real-world computational advantage. Nevertheless, the pedagogical clarity and ease of visualization make it a suitable and scalable starting point. Our future work will extend this framework to 3- and 4-qubit systems, leveraging cloud-based backends for hybrid simulation–execution pipelines.

2 Theoretical Framework

Grover's algorithm is a quantum search method that enables the location of a marked item within an unstructured database of N entries in $\mathcal{O}(\sqrt{N})$ queries, offering a quadratic speedup over classical brute-force approaches. This advantage is not domain-specific and stems from the quantum parallelism inherent in superposition and interference.

2.1 Problem Definition and Oracle Model

Let $f : \{0,1\}^n \to \{0,1\}$ be a Boolean function that evaluates to 1 for a unique marked element x^* and to 0 otherwise. The task is to find x^* using the fewest number of queries to f. Grover's algorithm assumes no structural information about f and operates under the black-box oracle model.

The quantum oracle O_f is constructed such that:

$$O_f|x\rangle = (-1)^{f(x)}|x\rangle,$$

which flips the phase of the marked state while leaving all others unchanged. In circuit terms, this can be implemented using controlled-Z or Toffoli-type gates, depending on the specific $f(x)$.

2.2 Amplitude Amplification Principle

The algorithm begins by preparing an equal superposition of all basis states:

$$|\psi\rangle = H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle.$$

The key innovation is the use of two reflections, first about the marked state via the oracle, and then about the average amplitude using the diffusion operator D:

$$D = 2|\psi\rangle\langle\psi| - I.$$

This pair of operations constitutes one **Grover iteration**, which rotates the system's state vector toward the solution. After $\mathcal{O}(\sqrt{N})$ iterations, the system is measured in the computational basis, yielding the target state x^* with high probability.

2.3 Geometric Interpretation

Grover's algorithm can be visualized geometrically in a two-dimensional Hilbert space spanned by the marked state $|x^*\rangle$ and its orthogonal complement. Each iteration rotates the state vector by a fixed angle θ, where $\sin(\theta/2) = 1/\sqrt{N}$. After $r \approx \frac{\pi}{4}\sqrt{N}$ iterations, the probability of measuring x^* is maximized. For small N, such as $N = 4$ in our 2-qubit simulation, only one Grover iteration is necessary to achieve perfect success (100% theoretical probability), assuming noiseless gates and perfect oracle construction.

2.4 Circuit Decomposition Strategy

Each component of Grover's algorithm, the Hadamard transform, oracle, and diffusion operator, =must be decomposed into native gates compatible with the target hardware. In IBM's Qiskit framework, this involves mapping abstract unitary operations to sequences of basis gates (typically $U3$, CX, and identity gates).

The diffusion operator for a 2-qubit system can be implemented using the sequence

1. Apply Hadamard gates to all qubits,
2. Apply Pauli-X gates to all qubits,
3. Use a controlled-Z gate to introduce conditional phase inversion,
4. Apply Pauli-X gates again, followed by Hadamards.

The oracle circuit depends on the marked item and can be systematically synthesized for any 2-qubit target using standard gate templates.

3 Methodology

This section outlines the practical implementation strategy adopted for simulating Grover's algorithm on a 2-qubit system. The methodology covers quantum circuit construction, oracle synthesis, noise modeling, and performance evaluation using IBM's Qiskit framework. All simulations were executed using Qiskit's Aer simulator, configured to reflect both ideal and noise-aware conditions.

3.1 Circuit Initialization and Oracle Construction

The simulation begins with the creation of an equal superposition state across $N = 4$ computational basis states using Hadamard gates applied to each qubit:

$$|\psi\rangle = H^{\otimes 2}|00\rangle = \frac{1}{2}\sum_{x=0}^{3}|x\rangle.$$

The oracle is designed to mark a specific target state $|x^*\rangle$ by applying a phase inversion. For the case $x^* = |11\rangle$, the oracle can be constructed using a combination of Pauli-X gates and a multi-controlled-Z operation, implemented via controlled-NOT and Z gates.

3.2 Grover Diffusion Operator

Following oracle application, the diffusion operator amplifies the amplitude of the marked state. For a 2-qubit system, the operator D is implemented using the following steps:

1. Apply Hadamard gates to all qubits,
2. Apply Pauli-X gates to all qubits,
3. Apply a controlled-Z gate to introduce a relative phase,
4. Reapply Pauli-X gates,
5. Reapply Hadamard gates.

This sequence completes one Grover iteration. For a 2-qubit system, a single iteration is theoretically sufficient to maximize the probability of measuring the target state.

3.3 Simulation Backends and Execution

The quantum circuit was executed using two primary backends provided by Qiskit Aer:

- **Statevector simulator**: Provides an ideal, noise-free representation of the final quantum state,
- **QASM simulator with noise model**: Includes measurement statistics and incorporates realistic device noise profiles.

Calibration data from IBMQ's real quantum devices were used to construct a custom noise model. Parameters such as T_1, T_2 coherence times, gate error rates, and readout errors were extracted using Qiskit's 'noise' module and applied to the QASM backend.

3.4 Performance Metrics

Two key metrics were used to assess the quality of the algorithm under noise:

1. **Success probability**: Defined as the fraction of measurement outcomes corresponding to the target state,

2. **Fidelity**: The overlap between the noisy state vector and the ideal, noiseless state.

Each simulation was repeated over 8192 shots to minimize statistical fluctuations. Results were plotted using Matplotlib and Seaborn, integrated into the Qiskit visualization pipeline.

4 Results and Discussion

In this section, we present the outcomes of simulating Grover's algorithm on a 2-qubit system. Both ideal and noise-influenced simulations were conducted to assess the performance and robustness of the algorithm under realistic conditions.

4.1 Ideal Case Simulation

Using the statevector simulator, we verified the correctness of the algorithm in the absence of noise. After a single Grover iteration, the final quantum state yielded the target basis state $|11\rangle$ with a theoretical probability of 1.0. The statevector output confirmed that all amplitude had been concentrated on the target state, validating both the oracle and diffusion implementations.

Measurement statistics from the QASM simulator under ideal conditions reflected this, with approximately 8192 out of 8192 shots yielding the target outcome $|11\rangle$, indicating no statistical error in simulation.

4.2 Noise Model Simulation

To emulate realistic hardware conditions, we incorporated a noise model based on calibration data from IBM's quantum devices. The noise model included gate errors, decoherence (via T_1 and T_2 times), and measurement inaccuracies.

Under this noise model, the success probability of measuring the correct output dropped significantly. Across 8192 trials, the mean frequency of the target outcome $|11\rangle$ was approximately 72 percent. The remaining 28 percent was distributed among the other basis states, primarily due to decoherence and gate errors.

4.3 Error Analysis and Interpretation

The performance degradation in the presence of noise highlights the vulnerability of shallow quantum circuits to real-world imperfections, even for small systems. In particular, we noted that:

- Gate infidelities contributed significantly to the dispersion of amplitude across incorrect states,
- Measurement errors caused occasional misclassification of the correct state,
- Coherence times imposed limitations on circuits with deeper Grover iterations.

These findings emphasize the importance of careful gate scheduling, qubit mapping, and error mitigation techniques when deploying quantum algorithms on near-term devices.

4.4 Educational and Practical Relevance

While the 2-qubit Grover algorithm is simple from a computational standpoint, its simulation under noise offers profound insights into the design principles required for scaling up quantum algorithms. The observed fidelity loss provides students and researchers with a tangible sense of the operational challenges in quantum computing.

Additionally, the simulation pipeline we have implemented is adaptable to arbitrary oracle functions and higher-dimensional Grover problems, enabling deeper exploration into quantum search and optimization on realistic hardware platforms.

5 Conclusion and Future Work

This work has demonstrated the implementation, simulation, and performance evaluation of Grover's algorithm on a 2-qubit system using IBM's Qiskit framework. By analyzing both ideal and noise-influenced simulations, we have illustrated the transition from theoretical quantum search to practical realization under realistic conditions.

The algorithm successfully amplified the amplitude of the target state in the absence of noise, confirming its expected theoretical behavior. However, under a noise model based on real quantum hardware calibration data, we observed a marked decline in success probability. This discrepancy highlights the limitations imposed by current Noisy Intermediate-Scale Quantum (NISQ) devices, especially when even minimal circuit depth is involved.

From an educational perspective, this project provides a scalable and reproducible workflow for early-stage researchers. The methodological clarity, combined with quantitative analysis, offers a foundation upon which more advanced implementations can be built. Instructors and learners alike can use this framework to better understand the implications of decoherence, gate errors, and readout inaccuracies on quantum algorithms.

Looking forward, several directions for future research emerge:

- **Extension to higher qubit counts**: Investigating Grover's algorithm on 3-qubit and 4-qubit systems will offer further insight into scalability and fidelity decay,
- **Oracle generalization**: Constructing oracles with multiple solutions and evaluating their performance across different noise models,
- **Error mitigation techniques**: Applying quantum error mitigation strategies, such as zero-noise extrapolation or dynamical decoupling, to improve performance on noisy backends,
- **Cross-platform benchmarking**: Implementing identical circuits on different quantum hardware platforms, such as IonQ and Rigetti, to compare their noise characteristics and algorithmic performance.

At last, while Grover's algorithm remains a pedagogically appealing and computationally significant quantum algorithm, its implementation on current quantum systems necessitates careful circuit design, realistic simulation, and ongoing optimization. This project serves as an initial yet meaningful step toward bridging the gap between textbook algorithms and practical quantum computing.

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