QUANTUM SEARCH AND CLASSICAL SEARCH

By

Ayush Raj Sethi

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ABSTACT

Quantum search represents one of the most influential breakthroughs in quantum algorithm design, offering a provable quadratic speedup over classical unstructured search. This thesis undertakes a comprehensive theoretical and experimental investigation of both classical and quantum search paradigms, focusing on Grover's Algorithm as the primary quantum model and linear search as the classical baseline. It explores the underlying mathematical foundations, circuit architecture, amplitude amplification dynamics, and the algorithm's convergence behaviour.

Unlike classical search, which requires an average of N/2 comparisons to locate a target in an unsorted dataset of size N, Grover's Algorithm exploits quantum superposition and interference to reduce the search time to $O(\sqrt{N})$. This acceleration is driven by the iterative application of two core operators: (1) the oracle, which marks the target by inverting its phase, and (2) the diffusion operator, which amplifies the probability amplitude of the marked state. A geometric interpretation reveals that each Grover iteration rotates the quantum state vector toward the target state within a two-dimensional Hilbert subspace.

To evaluate the algorithm's behaviour in practical environments, the study implements full quantum circuits using Qiskit's AerSimulator. Experiments analyse probability distributions, iteration counts, and measurement convergence across datasets ranging from 2 to 256 elements, comparing these outcomes with classical search performance. Additionally, the work presents detailed quantum circuit diagrams, benchmark graphs, and complete code listings.

The findings confirm consistency between theoretical predictions and simulation results: amplitude amplification occurs predictably, success probability increases sharply after successive iterations, and the number of required operations aligns closely with the theoretical $\pi/4\sqrt{N}$ bound. The thesis concludes by discussing limitations arising from classical simulation, lack of noise, and hardware constraints, while emphasizing the significance of Grover's Algorithm as an early demonstration of quantum advantage.

Chapter 1 — Introduction

The rapid growth of data generation in modern computational systems has highlighted the need for more efficient search algorithms capable of handling large unstructured datasets. Classical search methods, such as linear search, are limited fundamentally by their sequential nature, requiring O(N) time to locate a target element. This constraint becomes increasingly restrictive as datasets scale into millions or billions of entries. In contrast, quantum computing introduces a profoundly different computational paradigm that enables a dramatic reduction in search time through the exploitation of quantum mechanical principles.

Grover's Algorithm, introduced in 1996, stands as one of the most celebrated demonstrations of quantum computational advantage. Although not exponential like Shor's factoring algorithm, Grover's quadratic speedup is optimal for unstructured search problems. It provides a clear and mathematically provable improvement over classical techniques, making it a critical algorithm in understanding the practical potential of quantum computing.

1.1 Motivation for Research

The motivation behind investigating quantum search stems from current trends in computation: exponential data growth, increasing algorithmic complexity, and diminishing returns in classical hardware scaling. Quantum systems, with their inherent ability to represent and process multiple states simultaneously, offer a compelling approach for future-proof algorithm design. By studying Grover's Algorithm in detail—mathematically, architecturally, and experimentally—this thesis aims to provide foundational insights relevant to students and researchers in the field of quantum information science.

1.2 Research Objectives

The primary objective of this research is to perform a rigorous comparative analysis of classical linear search and Grover's Quantum Search Algorithm from theoretical, architectural, and experimental viewpoints. The study aims to bridge the gap between high-level algorithmic descriptions and practical implementations using modern quantum simulation frameworks. To achieve this overarching goal, the following specific research objectives are defined:

1. **Formulate a detailed mathematical foundation** for Grover's Algorithm, including amplitude amplification, oracle construction, diffusion operator analysis, and geometric rotation interpretation within a reduced Hilbert subspace.
2. **Develop complete quantum circuit implementations** using Qiskit, incorporating multi-controlled gates, oracle logic synthesis, and amplitude amplification blocks aligned with theoretical constructs.
3. **Implement classical linear search algorithms** as a computational baseline, enabling a controlled comparison between classical O(N) and quantum O(√N) runtimes.

4. **Design and execute comprehensive simulation experiments**, evaluating probability distributions, iteration behaviour, measurement convergence, and circuit-level performance across increasing problem sizes.
5. **Analyse benchmark results quantitatively**, comparing classical steps, quantum iterations, theoretical speedup factors, and success probabilities under ideal simulation conditions.
6. **Identify limitations and constraints** inherent in classical simulation of quantum algorithms, including scalability bottlenecks, gate depth restrictions, and the absence of decoherence effects.
7. **Provide reproducible appendices and circuit schematics** that allow future researchers to extend or replicate the study.

1.3 Structure of the Thesis

To maintain clarity and coherence, the thesis is organized into the following major chapters:

- **Chapter 2:** Provides foundational quantum computing concepts.
- **Chapter 3:** Derives the mathematical framework of Grover's Algorithm.
- **Chapter 4:** Discusses classical search and computational constraints.
- **Chapter 5:** Presents quantum circuit architecture and component design.
- **Chapter 6:** Details the simulation environment and experimental setup.
- **Chapter 7:** Evaluates results with probability graphs and benchmark tables.
- **Chapter 8:** Discusses implications, limitations, and theoretical considerations.
- **Chapter 9:** Summarizes findings and outlines future research directions.

1.4 Scope and Limitations

This study focuses specifically on unstructured search problems and idealized quantum conditions. Real quantum hardware introduces noise, decoherence, and limited qubit connectivity—factors not present in classical simulations. Therefore, the presented results should be viewed as theoretical upper bounds on Grover's performance. Expanding beyond these bounds requires specialized hardware or error-corrected quantum systems, which remain in early development.

Chapter 2 — Background

Quantum computing is fundamentally rooted in the mathematical formalism of linear algebra and the physical principles of quantum mechanics. Unlike classical bits that assume definite binary values from the set {0,1}, quantum bits (qubits) inhabit a continuous state space defined over complex amplitudes. A single qubit can be expressed as a vector in a two-dimensional Hilbert space:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$\text{where } \alpha,\beta \in \mathbb{C} \text{ and } |\alpha|^2 + |\beta|^2 = 1$$

This representation allows for *superposition*, one of the foundational phenomena enabling quantum algorithms to outperform classical ones. When extended to n qubits, the state space grows exponentially to 2^n dimensions, enabling simultaneous representation of all computational basis states.

Another key property is *entanglement*, a non-classical correlation between qubits that permits global transformations without independent manipulation of individual subsystems. Entanglement enables powerful algorithmic constructs such as quantum teleportation, Shor's factoring algorithm, and key components of Grover's search.

Quantum computation proceeds through *unitary evolution*, where transformations are applied through quantum gates represented by unitary matrices ($U^\dagger U = I$). Unlike classical logic gates that may destroy information, unitary operations are reversible, requiring careful circuit planning. Measurement collapses superpositions into classical outcomes, introducing probabilistic behaviour into computations.

Quantum algorithms gain efficiency by structuring these phenomena into constructive interference patterns, routing amplitude toward correct solutions while diminishing amplitude elsewhere. Grover's algorithm stands as the most elegant demonstration of this principle.

Chapter 3 — Quantum Computing Foundations

Quantum computation relies on mathematical constructs from linear algebra, complex vector spaces, and operator theory. This chapter presents the foundational concepts required to understand Grover's algorithm at a formal level.

3.1 Qubit Representation and Multi-Qubit Systems

A single qubit is represented as a linear combination of the computational basis states:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \text{ with } |\alpha|^2 + |\beta|^2 = 1$$

For a system of *n* qubits, the joint state is represented using the tensor product (⊗):

$$|\psi\rangle = |q_1\rangle \otimes |q_2\rangle \otimes \dots \otimes |q_n\rangle$$

leading to a 2^n-dimensional state vector. This exponential state growth underlies the power of quantum computation.

3.2 Unitary Operators and Reversible Computation