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Quantum Optimization for Enhanced Combinatorial Algorithms

Pradeep Kumar Pandey, Ruchi Chaturvedi, Suraj Bhan Dangi*

Department of Computer Science & Technology, Sam Global University, Raisen, Madhya Pradesh, India

ABSTRACT

The twenty-first century has been the era of data. Algorithms are crucial in tasks ranging from simple document searches to complex batching and scheduling jobs. Optimization techniques are often applied to enhance algorithms and achieve better results. As Moore rightly predicted, the exponential increase in transistors has led to a point where classical computers can no longer solve specific problems within a human timeframe. This paved the way for the development of quantum computers, which utilize quantum phenomena to solve problems. Quantum optimization techniques and algorithms have been designed to leverage the quantum advantage for improved optimization. This research compares and presents the results of quantum optimization techniques applied to classic combinatorial algorithms.

Keywords: *Quantum Optimization, Combinatorial Algorithms, Quantum Computing, Algorithm Efficiency, Computational Complexity*

1. Introduction

Quantum computers utilize quantum phenomena to execute various computations [1]. Quantum advantage primarily depends on two factors: first, the quantum computer itself, and second, the algorithms developed to leverage these quantum phenomena. The fundamental component of a quantum computer is known as a qubit. Qubits are said to exist in a superposition of two states: the off state (0) and the on state (1). Unlike a classical bit, which can be either in a 0 state or a 1 state, a qubit can be in both states simultaneously at the exact moment. This property allows n qubits to represent 2^n states at once.

Quantum computing relies on three main quantum properties of an atom:

i. Superposition
ii. Entanglement
iii. Interference

Superposition is the property that allows atoms to exist in multiple states simultaneously. This property enables quantum computers to scale and perform exponentially better than classical computers. Entanglement is the phenomenon where two atoms remain correlated, even when separated by vast distances [2]. This property facilitates the instantaneous transfer of information. Interference is the process by which an atom collapses from a superposition into a single state when it interacts with its environment. Interference plays a crucial role in information security, as even a small disturbance can cause the collapse of an atom's superposition state [3]. Another key phenomenon in quantum computing is quantum entanglement, which enables qubits to be intrinsically linked, regardless of distance. When entangled, the state of one qubit instantly determines the state of another, providing a means for highly efficient information transfer and parallel computation [4]. These quantum properties facilitate the execution of quantum algorithms such as Shor's algorithm for integer factorization, which threatens conventional cryptographic security, and Grover's algorithm for searching unstructured databases exponentially faster than classical algorithms [5][6]. Quantum advantage, the point at which a quantum computer surpasses classical systems in problem-solving efficiency, depends on the hardware and algorithms designed to exploit quantum mechanics effectively. Developing quantum algorithms and error correction techniques is crucial for practical quantum computing applications. Current implementations of quantum computers include: superconducting qubits, trapped ions, and topological qubits, each offering distinct advantages and challenges regarding coherence time, scalability and noise resistance [7]. Despite significant advancements, quantum computing still faces considerable challenges, including qubit decoherence, error rates, and the need for large-scale fault tolerance [8]. Researchers continue to explore novel materials, quantum error correction codes, and hybrid quantum-classical algorithms to enhance the feasibility and scalability of quantum computing [9].

Our study focuses on applying the Quantum Approximate Optimization Algorithm (QAOA) to classical combinatorial problems such as: Max-Cut and Knapsack Problem, demonstrating its effectiveness in achieving optimized solutions. Using these quantum principles, the QAOA is used as a promising method for solving classical combinatorial problems like Max-Cut and the Knapsack problem. This study evaluates QAOA's effectiveness in finding optimized solutions and compares its advantages with classical techniques. By bridging classical and quantum optimization, it helps improve our understanding of quantum algorithms in problem-solving. Additionally, this research lays the groundwork for future studies by comparing QAOA with other quantum methods and benchmarking them against classical approaches.

1.1 Optimization

Optimization for any algorithm can be of two types: (1) Arriving at a solution that is closest to the expected result, and (2) the amount of time taken to arrive at the solution.

*Corresponding author:surajdangisd97@gmail.com

Below are some of the commonly used quantum optimization techniques for computing problems.

1.2 Quantum Annealing

Quantum annealing, or Quantum Stochastic Optimization, is an optimization technique that allows us to find the global minimum for functions with several local minima. Quantum annealing uses two main techniques to achieve its goal: (i) quantum fluctuations and (ii) quantum tunneling. Quantum fluctuations refer to the change in the energy level of a qubit by an external magnetic field which allows it to end up in the lowest energy level. This quantity that controls the magnetic field is called bias [10]. Quantum tunneling helps qubits propagate through potential barriers instantaneously without climbing them. These factors prove quantum annealing is more efficient and faster to converge to the optimal solution [11].

1.3 Quantum Approximate Optimization Algorithm (QAOA)

QAOA is an optimization technique that is used to solve combinatorial optimization problems like the NP-Hard Max-cut problem. The aim of the max cut problem is to obtain a value close to the maximum no. of edge cuts (C) possible in a given graph (G). Classical function with binary variables is encoded by introducing a quantum spin for each variable. QAOA has proven to be more efficient than the classical technique in arriving at the closest solution [12].

1.4 Adiabatic Quantum Optimization

Adiabatic Q-optimization aims to find the optimal solution by evolving the ground state rapidly. Similar to quantum annealing, this technique also starts with a Hamiltonian ground state. Unlike quantum annealing, which uses quantum tunneling to pass through states that might end up in a local minimum, this adiabatically evolves and arrives at the optimal solution [13,14].

2. Methodology

QAOA Implementation: The QAOA is a hybrid quantum-classical algorithm designed to solve combinatorial optimization problems efficiently. It operates by iteratively optimizing a quantum circuit parameterized by classical optimization techniques. Our implementation of QAOA includes several crucial aspects:

2.1 Parameter Selection

The QAOA performance heavily depends on the selection of variational parameters β and γ, which control the evolution of the quantum state. We employed gradient-based and heuristic optimization methods, such as Nelder-Meadand COBYLA, to fine-tune these parameters.

2.2 Circuit Design:

The quantum circuit for QAOA consists of alternating layers of problem Hamiltonian evolution and mixing Hamiltonian evolution. We used a depth parameter "*p*" to control the number of layers, balancing accuracy and quantum resource constraints.

3. Proposed Work

3.1 MAX CUT

Max–Cut problem is a classical NP-Hard problem that tries to find the maximum cut which splits the graph into two sets that would have the greatest number of edges in between it [9]. QAOA is a quantum algorithm that leverages the use of quantum properties to arrive at an optimized approximate solution. QAOA is a heuristic algorithm that provides the closest answer in polynomial time. The algorithm does not guarantee performance but is expected to produce a result closest to the actual solution [10]. The circuit for finding the Maximum-Cut of the graph starts by placing all the qubits in superposition. This becomes the initial state. A unitary is applied to the circuit according to the Hamiltonian for the graph. Later, a mixing unitary is applied. Optimal parameters for the circuit are initialized using a classical optimization algorithm, which is then applied to a QAOA circuit. Steps are repeated until convergence is achieved.

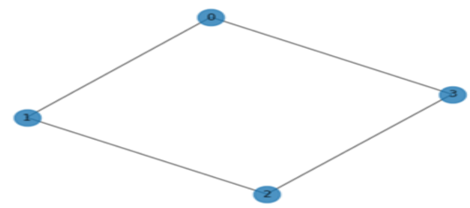


Fig. 1 Graph with 4 nodes

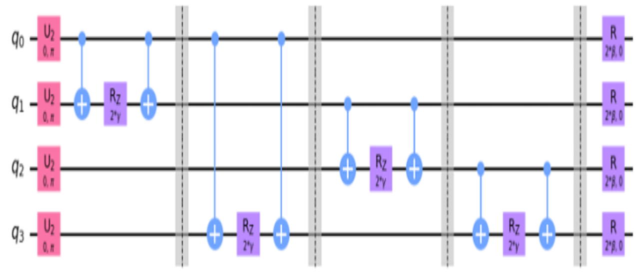


Fig. 2 Circuit for solving using QAOA

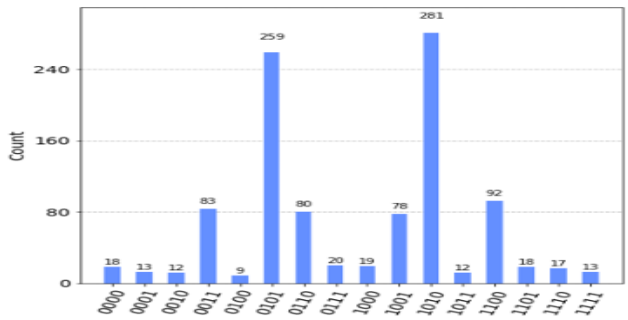


Fig. 3 Results for Max-Cut with 4 nodes

QAOA also guarantees to achieve the most optimal solution for weighted Max-Cut problems. Here a Hamiltonian model of the weighted graph is generated which is then applied to the QAOA to find the maximum cut [7].

3.2 Knapsack Problem

The Knapsack problem is an NP-complete problem that involves combinatorial optimization. The problem involves finding the set of items that give the maximum value for a given knapsack weight. The problem has two flavors; one is the 0-1 Knapsack problem that only allows to add only one copy of an item. The bounded knapsack allows many copies of an item but restricts it to an upper bound. The quantum optimization for Knapsack is carried out using QAOA. The circuit is first initialized to superposition. Hamiltonian is constructed for the problem. The Hamiltonian is solved using the Minimum Eigen Optimizer. Thus, the result is obtained by finding the maximum value of the objective function.

Table 1 Max Cut Results using QAOA

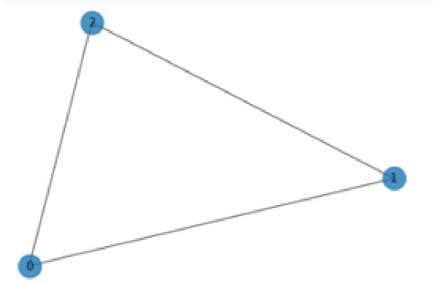
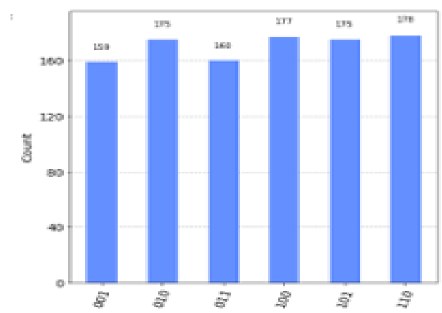
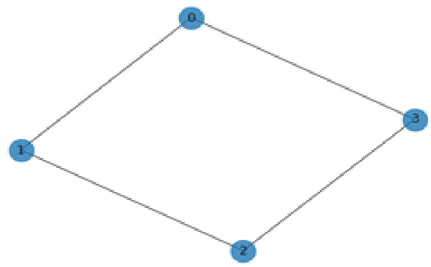
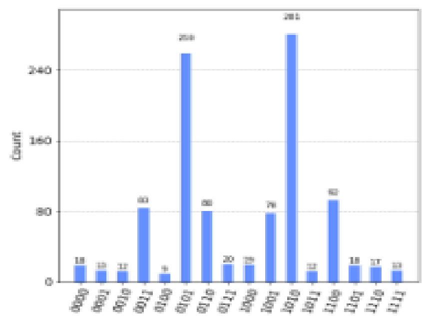
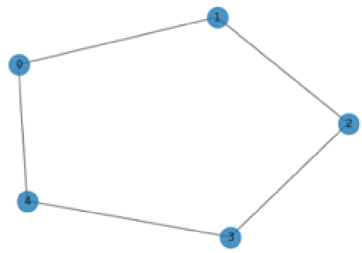
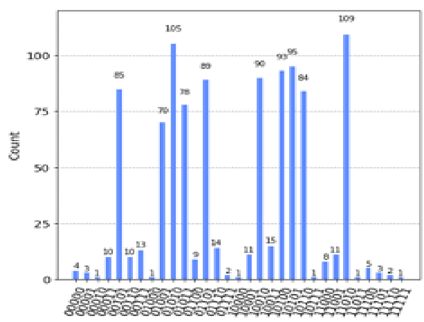
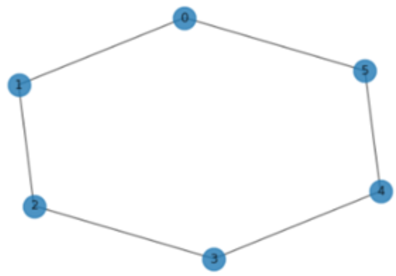
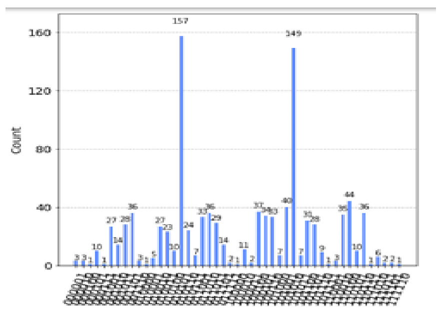
No of Nodes	Graph	Max-Cut Solution using QAOA
3		
4		
5		
6		

Table 2 Knapsack Results using QAOA

No. of items	Values	Maximum Weight of Knapsack	Weights	Objective function (Max Z)	Solution	Time taken (s)
5	[3, 4, 5, 6, 7]	10	[2, 3, 4, 5, 6]	$3^*x\_0 + 4^*x\_1 + 5^*x\_2 + 6 x^*x\_3 + 7^*x\_4$	[0, 1, 3]	4.285
6	[3, 4, 5, 6, 7,8]	12	[2, 3, 4, 5, 6,7]	$3^*x\_0 + 4^*x\_1 +5^*x\_2 + 6^*x\_3 + 7^*x\_4 +8^*x\_5$	[0, 2, 4]	1.241
7	[3, 4, 5, 6, 7,8,2]	15	[2, 3, 4, 5, 6,7,10]	$3^*x\_0 + 4^*x\_1 +5^*x\_2 + 6^*x\_3 + 7^*x\_4 +8^*x\_5 \; 2^*x\_6$	[0, 1, 2, 4]	11.46

4. Advantages of Quantum Optimizers over Classical Optimizers

Quantum computing leverages superposition, allowing quantum bits (qubits) to exist in multiple states simultaneously rather than being confined to a single binary state like classical bits. This capability significantly enhances computational power, enabling the exploration of many possible solutions in parallel before arriving at an optimal result. For combinatorial optimization problems, this property provides a key advantage, as it allows quantum algorithms to evaluate numerous potential solutions efficiently. These problems are first mathematically modelled using a Hamiltonian function, representing the system's total energy, encoding the constraints and objectives of the optimization problem. Once the problem is formulated in this manner, Quantum optimizers are employed to find the best solution. Quantum optimizers are generally categorized into two types:

4.1 Heuristic-based optimization:

These methods use probabilistic and approximation techniques to explore the solution space and converge toward the most optimal solution. Examples include QAOA and the variational quantum Eigen solver (VQE).

4.2 Performance-based optimization:

These techniques focus on reducing time complexity, leveraging quantum speedup to solve problems faster than their classical counterparts. Algorithms such as Grover's search or quantum annealing fall into this category, enabling more efficient computations for large-scale problems.

By integrating these optimization strategies, quantum computing presents a promising alternative to classical approaches, particularly for complex combinatorial problems that require evaluating many possible solutions within a feasible timeframe. By incorporating these optimization strategies, quantum computing emerges as a promising alternative to classical approaches, particularly for solving complex combinatorial problems that involve evaluating a vast number of possible solutions within a feasible timeframe.

5. Conclusion

This research explores the potential of the QAOA in solving classical combinatorial problems such as the Max-Cut and Knapsack Problem, both of which are fundamental in optimization and have wide-ranging applications in fields like logistics, finance, and network design. Our study demonstrates that QAOA effectively provides optimized solutions for these problems by leveraging quantum superposition and entanglement to explore multiple solution spaces simultaneously. QAOA consistently achieves near-optimal results across various problem instances through iterative circuit optimization and variational parameter tuning. Despite its promising performance, the effectiveness of QAOA is influenced by factors such as quantum hardware noise, decoherence, and the selection of variational parameters. These challenges highlight the necessity for further refinement in quantum error mitigation and hybrid classical-quantum optimization techniques to improve their scalability and real-world applicability. Additionally, the depth of the QAOA circuit plays a crucial role in the accuracy of the solution, requiring a balance between computational complexity and hardware constraints.

6. Future Scope

Future research could extend this work by applying QAOA to a broader range of combinatorial problems, such as the Traveling Salesman Problem and Graph Partitioning, to assess its effectiveness across diverse optimization landscapes. Comparative studies with alternative quantum optimization methods, including Quantum Annealing and Variational Quantum Eigen solver VQE, could provide deeper insights into the relative advantages of different approaches. Further exploration into hybrid quantum-classical strategies, improved error mitigation techniques, and scalability analysis will be essential for enhancing the feasibility of QAOA on near-term quantum hardware. Moreover, testing QAOA across various quantum architectures, such as superconducting qubits, trapped ions, and photonic quantum systems, may uncover hardware-specific optimizations that improve performance. These directions will help advance quantum optimization techniques closer to practical real-world applications.

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