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Research Project – Topic Brief

Quantum Optimization for the Vehicle Routing Problem (VRP)

1. INTRODUCTION

The Vehicle Routing Problem (VRP) is a fundamental combinatorial optimization challenge in logistics, aiming to determine the most efficient routes for a fleet of vehicles to service a set of customers. Over the years, VRP and its different versions have become a popular topic in research. However, since the problem can be defined in many versions (many ways with many different assumptions), researchers need to be aware that VRP itself has a broad range of variants [1]. Given its NP-hard nature, classical algorithms often struggle with large-scale instances due to computational limitations.

The City of Casey provides detailed datasets on waste facilities, public litter bins, and collection areas, making it an ideal case study for applying Vehicle Routing Problem (VRP) optimization techniques. By integrating real-world constraints such as traffic conditions, weather, and road incidents, this study models a practical VRP instance. With the problem's NP-hard nature, classical approaches face computational challenges in large-scale optimization.

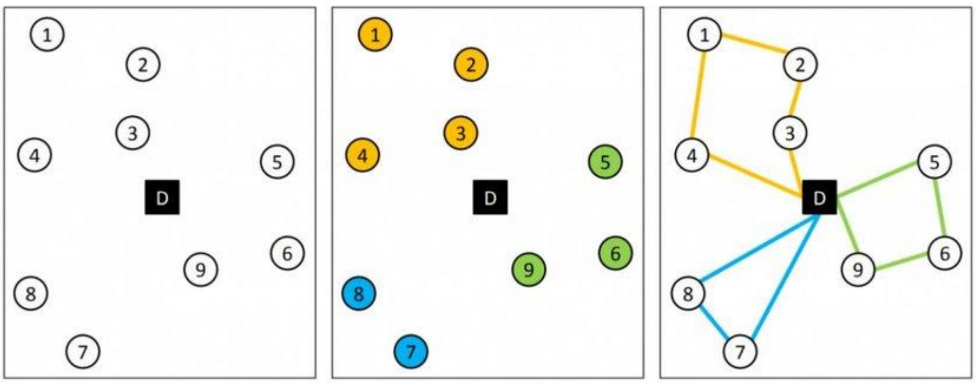
Quantum computing offers a paradigm for approaching and solving such problems. Algorithms like the Quantum Approximate Optimization Algorithm (QAOA) [2] and Quantum Walk-based Optimization [3] have shown promise in tackling NP-hard tasks. This research proposes to explore these quantum techniques to develop efficient approximation methods for the VRP.

2. SCOPE AND BOUNDARIES

2.1 Vehicle Routing Problem

VRP has numerous real-world applications, including logistics, supply chain management, and last-mile delivery services. Various VRP variants exist, such as the Capacitated VRP (CVRP), Time-Window VRP (VRPTW), and Stochastic VRP (SVRP), each introducing unique constraints that impact solution complexity. Classical methods struggle to find optimal solutions as problem size increases due to exponential computational growth.

This diagram is one method of finding solution to VRP [4]:



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Unassigned Customers (Left Panel)

- Customers (represented by numbered circles) are scattered around a central depot (black square labeled "D").
- At this stage, no routes have been assigned.

Customer Clustering (Middle Panel)

- Customers are grouped into different sets based on their locations and other factors such as demand or distance (this is where heuristic comes into play).
- Each color represents a different vehicle that will serve a specific group (with certain heuristics) of customers.

Optimized Routes (Right Panel)

- Vehicles are assigned optimized routes that start and end at the depot (D).
- Each route ensures that all customers are served efficiently while minimizing travel distance and cost.

2.2 Case Study: Waste Collection in the City of Casey

To analyze the Vehicle Routing Problem (VRP) in a practical setting, we consider a case study based on real-world waste collection services. The waste collection scenario is chosen due to its public, detailed, and structured dataset. The study focuses on the City of Casey, as this place offers granular data, an ideal dataset for modeling and validating VRP solutions.

The VRP model is constructed based on three key components: depots, customers, and routes:

- **Depots**
  Waste collection facilities serve as depots [5], where vehicles begin and end their routes
- **Customers**
  Public litter bin locations represent customer nodes [6], where waste collection must be performed and combined with waste collection area data for comprehensive coverage [7], ensuring a comprehensive mapping of all waste pickup points across the city
- **Routes**
  Based on Victoria's road network [8], paths for vehicle travel between depots and collection points

To enhance the model's accuracy and reflect real-world complexities, additional constraints can be introduced:

- Traffic: Higher traffic increases travel time [9]
- Weather (Rainfall): More rainfall slows travel [10]
- Road Crashes: Accidents cause delays [11]

2.3 Quantum Optimization

Quantum computing offers a novel approach to solving VRP by leveraging quantum superposition and entanglement to explore multiple solutions simultaneously. Quantum algorithms like QAOA and Quantum Walk-based methods have shown potential in improving combinatorial optimization efficiency. However, implementing these algorithms for practical VRP scenarios requires addressing efficiency, scalability, and quantum hardware limitations.

3. BACKGROUND AND CHALLENGES

3.1 Classical Approaches to VRP

Traditional methods for solving the VRP include:

- Exact Algorithms: Techniques such as Branch-and-Bound for CVRP [12]
- Metaheuristic Approaches: Algorithms like Genetic Algorithms (GA) and Ant Colony Optimization (ACO) offer approximate solutions more feasibly but may not guarantee optimality [13]

3.2 Quantum Programming Approaches to VRP

Quantum Optimization Techniques can offer a better solution than a classical one. Several approaches have been proposed to explore the advantages of quantum algorithms over classical optimization methods, particularly for NP-hard problems like the Vehicle Routing Problem (VRP):

- Quantum Approximate Optimization Algorithm (**QAOA**): QAOA is designed to find approximate solutions to combinatorial problems by leveraging quantum superposition and entanglement [14].
- **Quantum Walk-based Optimization**: Quantum walks, the quantum analog of classical random walks, have been applied to search and optimization problems, offering potential speedups over classical methods [15].
- Variational Quantum Eigensolver (**VQE**): VQE is another quantum algorithm that has been studied for solving VRP. Currently, Noisy-Intermediate Scale Quantum (NISQ) devices can only handle small VRP instances, but as quantum hardware improves, both VQE and QAOA are expected to perform better and potentially surpass classical methods [16].
- **Quantum Annealing**: A novel Quadratic Unconstrained Binary Optimization (QUBO) formulation has been proposed for the Capacitated Vehicle Routing Problem (CVRP), incorporating a time-table representation to model the time evolution of each vehicle. This formulation successfully integrates time-based and capacity constraints, allowing for dynamic updates as vehicles visit different cities [17].

In this study, we will compare the performance of quantum optimization algorithms in solving VRP instances. We will simulate quantum circuits and benchmark them against classical methods to assess their potential advantages in solving complex routing problems.

4. PROPOSED RESEARCH OBJECTIVES

1. Develop quantum optimization approaches for VRP (in this case, waste collection) using Quantum Algorithms.
2. Compare quantum and classical algorithms by analyzing solution quality, computational efficiency, and scalability.
3. Investigate the effectiveness of quantum approximations in solving VRP and their ability to find near-optimal solutions.
4. Implement a quantum-based VRP solution with the potential to outperform classical methods in specific scenarios.

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5. RESEARCH QUESTIONS

All of the discussion leads to research that needs to be done which includes around these four questions:

RQ1. How can spatial datasets be transformed into a VRP formulation suitable for quantum optimization?
RQ2. How can quantum optimization techniques such as QAOA, Quantum Walk, VQE, and/or Quantum Annealing provide a more effective solution for VRP compared to classical methods?
RQ3. In terms of efficiency and scalability, how do quantum algorithms compare to state-of-the-art classical VRP solvers?
RQ4. What are the key limitations of using quantum algorithms for VRP, and how can these challenges be addressed?

6. LITERATURE REVIEW

The Vehicle Routing Problem (VRP) is a well-known NP-hard problem that has been extensively studied in logistics and supply chain management. Given the computational complexity of VRP, researchers have explored various quantum optimization approaches, including the Quantum Approximate Optimization Algorithm (QAOA), Quantum Walks, and Quantum Annealing, to improve efficiency and scalability.

6.1 Quantum Approximate Optimization for VRP

QAOA is useful for VRP because it can efficiently find approximate solutions to complex optimization problems, including route planning. VRP involves selecting the best paths for multiple vehicles while considering constraints like distance, capacity, and time windows. Since VRP is an NP-hard problem, classical algorithms struggle to solve large instances efficiently. QAOA leverages quantum superposition and interference to explore multiple possible solutions simultaneously, potentially finding good routes faster than classical heuristics.

Mathematically, QAOA encodes the VRP as a cost function H_C, which represents the total travel distance or other constraints, and a mixing function H_M , which helps the algorithm explore different routes. The quantum circuit is defined as:

$$|\psi(\gamma, \beta)\rangle = U_M(\beta_p)\, U_C(\gamma_p) \ldots U_M(\beta_1)\, U_C(\gamma_1)\, |s\rangle$$

where $U_C(\gamma) = e\text{\^{}}(-i\gamma H_C)$ encodes the VRP constraints, and $U_M(\beta) = e\text{\^{}}(-i\beta H_M)$ allows transitions between different solutions. Fitzek et al. [18] applied this method to handle vehicle-specific constraints, improving efficiency. Leonidas et al. [19] optimized QAOA for small quantum devices by reducing qubit requirements. Farhi et al. [14] originally introduced QAOA, showing that deeper circuits can improve results, though real quantum hardware still has limitations.

6.2 Quantum Walk-based Approaches

Quantum walks, which serve as a quantum analog to classical random walks, have been explored for VRP optimization. Quantum walks are useful for VRP because they can explore large search spaces efficiently by leveraging quantum interference and superposition. Unlike classical random walks, where the probability of moving to a new state depends only on the previous step, quantum walks maintain phase coherence, allowing for faster propagation through the solution space. The evolution of a discrete-time quantum walk is governed by the unitary operator:

$$U = S \cdot (I \otimes C)$$

where S is the shift operator that moves the walker between states, and C is the coin operator that controls the direction of movement. Bennett et al. [15] applied this framework to vehicle routing, demonstrating that quantum walks can help find optimal paths by efficiently traversing possible routes. Marsh and Wang [20] introduced an approximation method based on quantum walks, showing its applicability to bounded NP-hard problems. In a later study, they improved the efficiency of combinatorial optimization by refining the quantum walk formulation to enhance solution quality [21]. These works suggest that quantum walks could provide speedups for VRP compared to classical heuristics, though practical implementation remains limited by current quantum hardware constraints.

6.3 Quantum Annealing for VRP

Quantum annealing has been another area of research in VRP optimization. Tambunan et al. (2023) investigated quantum annealing for VRP with weighted segments, focusing on integrating dynamic constraints within the optimization process [22]. Similarly, Irie et al. (2019) formulated a Quadratic Unconstrained Binary Optimization (QUBO) model for VRP with time, state, and capacity constraints, showcasing quantum annealing's applicability in complex routing scenarios [17].

Quantum annealing (QA) is a heuristic algorithm used for solving optimization problems, including the Vehicle Routing Problem (VRP). It relies on the principle of quantum mechanics, specifically the quantum superposition and tunneling phenomena, to find the global minimum of a cost function. In the context of VRP, the cost function typically represents the total travel distance or time, incorporating constraints such as vehicle capacity, time windows, and traffic conditions. QA starts with an initial Hamiltonian that describes the problem's configuration and evolves this system toward a final Hamiltonian that encodes the solution. The objective is to find the ground state of this system, which corresponds to the optimal solution. The general form of a Hamiltonian used in quantum annealing for VRP can be expressed as:

$$H(t) = A(t)H_p + B(t)H_D$$

where H_p is the problem Hamiltonian that encodes the VRP objective and constraints, and H_D is the driver Hamiltonian that governs the evolution of the quantum state. The functions A(t) and B(t) control the mixing between these Hamiltonians during the annealing process. As the annealing progresses, the system ideally transitions into the lowest energy state, providing a solution to the VRP. Recent studies, such as those by Irie et al. [17] and Tambunan et al. [22], demonstrate the viability of quantum annealing in addressing complex VRP instances with dynamic and weighted constraints, highlighting its potential as a tool for optimization in real-world logistics applications.

6.4 Hybrid and Machine Learning Approaches

Beyond traditional quantum techniques, researchers have explored hybrid quantum-classical methods and machine learning integration for VRP. Hybrid quantum-classical methods, such as Quantum Support Vector Machines (QSVMs) and Variational Quantum Algorithms (VQAs), offer promising approaches to solving the Vehicle Routing Problem (VRP) by leveraging the strengths of both quantum computing and classical optimization. In the case of QSVM, the algorithm aims to classify routes by transforming the VRP into a classification problem. The kernel function in QSVM is typically quantum-enhanced, offering the potential to process high-dimensional data more efficiently than classical methods. The decision function for QSVM is given by:

$$f(x) = \mathrm{sgn}(\sum \alpha_i y_i \langle \phi(x_i) | \phi(x) \rangle + b)$$

where $\langle \phi(x_i) | \phi(x) \rangle$ represents the inner product between quantum states, and α_i and b are parameters determined through training. This approach enhances the accuracy of route classification, improving overall VRP optimization. On the other hand, VQAs utilize parameterized quantum circuits in combination with classical optimization algorithms to iteratively adjust quantum states and minimize the objective function. The quantum circuit's parameters are adjusted using a classical optimizer to solve for the optimal routing decisions under given constraints. These hybrid methods take advantage of quantum computing's potential for high-dimensional state space exploration, while maintaining practical feasibility in hardware-limited environments, as demonstrated by Alsaiyari and Felemban [16] and Mohanty et al. [23].

The exploration of quantum algorithms for VRP has revealed promising directions, particularly with QAOA, quantum walks, and quantum annealing. While current research demonstrates theoretical advantages over classical methods, practical implementations remain limited by hardware constraints. Future work should focus on improving qubit efficiency, hybrid algorithm designs, and benchmarking against state-of-the-art classical solvers to fully leverage quantum optimization for large-scale VRP applications.

7. PROPOSED METHODOLOGY

7.1 Quantum Computing Approaches

- Formulation: Represent the VRP in a quantum framework suitable for QAOA, Quantum Walk algorithms, and VQE.
- Theoretical Calculations: Analyze mathematical models and complexity to understand how quantum algorithms can outperform classical methods in VRP domain. This includes identifying cases where quantum optimization provides faster solutions or better approximations.
- Implementation: Develop and simulate quantum circuits using platforms like PennyLane or Qiskit (or other compatible library)

7.2 Benchmarking Strategy

- Classical Comparison: Utilize established solution using classical methods to obtain baseline solutions.
- Performance Metrics: Compare quantum and classical approaches based on solution quality, computational time, and scalability.

7.3 Datasets

- Data Acquisition: Employ real-world datasets from public sources.

- Data Processing: Transform raw data into graph representations that will be compatible with quantum algorithms.

8. EXPECTED OUTCOMES, CONTRIBUTIONS, AND CHALLENGES

8.1 Expected Outcomes and Contributions

- Development of quantum-based approximation methods: Providing new strategies for solving VRP using quantum computing.
- Comparative Analysis: Offering insights into the practical advantages and limitations of quantum versus classical approaches for VRP.

8.2 Challenges and Limitations

Quantum Hardware Constraints: Real quantum cloud is expensive. Use a simpler graph to simulate in real quantum computer and use a simulator to simulate bigger graph.

9. APPROXIMATE TIMELINE

9.1 First Semester (50 Points)

- Week 1: Topic Formulation
    - Finalize research topic and objectives.
    - Output: Topic finalized by end of week 1.
- Week 2-4: Literature Review
    - Explore quantum algorithms and circuits (QAOA, Quantum Walk, VQE, Quantum Annealing)
    - Review existing research on quantum optimization for VRP
    - Output: Gain more hands-on experience with quantum algorithms.
- Week 5-6: Research Methodology Formulation
    - Develop research methodology to approach VRP using quantum optimization.
- Week 7-8: Research Proposal Drafting
    - Write research proposal with objectives, methodology, and case study specifics.
    - Output: Research proposal submitted by end of week 8.
- Week 9-11: Data Acquisition
    - Collect data from real-world sources (City of Casey waste collection, road networks, etc.).
    - Output: Structured dataset for VRP.
- Week 11: Oral Presentation
    - Prepare and deliver a 10-15 minute oral presentation on research progress
- Week 12: Continue with Quantum Algorithm Formulation

9.2 Second Semester (50 Points)

- Week 1-3: Data Translation (Spatial to VRP Graph)
    - Translate spatial data into a VRP-compatible graph
    - Output: Transformed VRP data representation.

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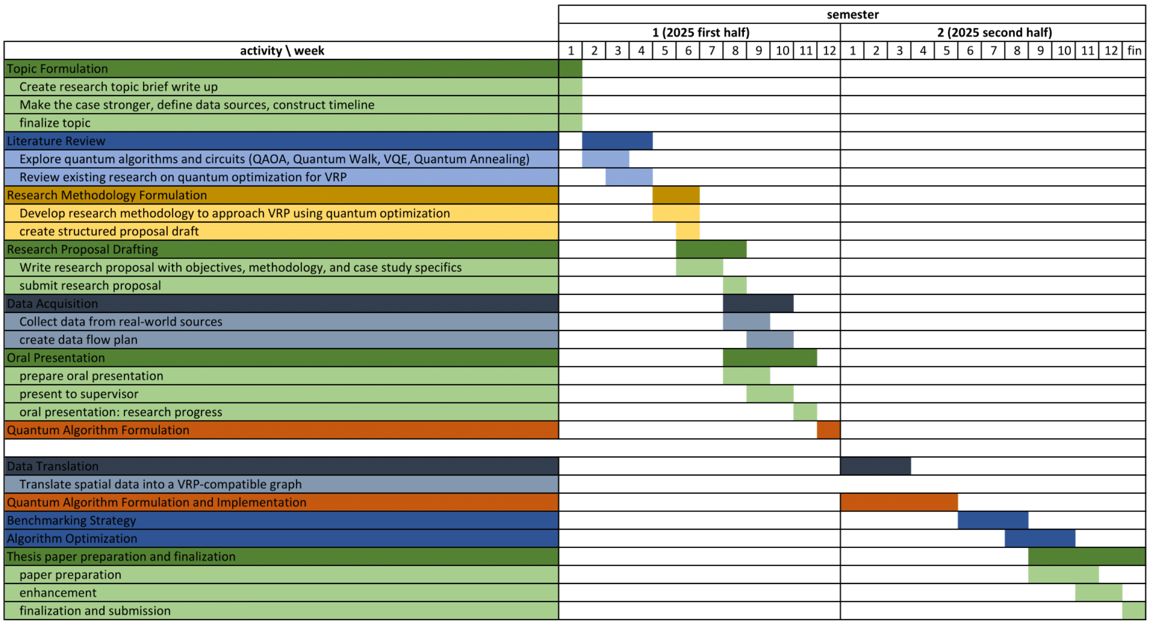
- Week 1-5: Quantum Algorithm Formulation
  - Develop quantum optimization algorithms (QAOA, Quantum Walk) for VRP.
  - Start with basic formulations and progress to complex VRP instances.
  - Output: Working quantum algorithms.
- Week 6-8: Benchmarking Strategy
  - Design a strategy to compare quantum optimization results with classical algorithms.
  - Collect performance metrics (solution quality, computational time, scalability).
- Week 8-10: Algorithm Optimization
  - Refine quantum algorithms to improve performance and scalability.
- Week 11-12: Thesis Defense
  - Final Week: Thesis Submission
  - Output: Complete and submit a written thesis (25,000-30,000 words).



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