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Quantum Algorithms for Optimizing Urban Transportation

Bruno André Moreira Rosendo

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Supervisor: Rui Maranhão

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Abstract

Transportation is a fundamental aspect of modern urban life, profoundly influencing the daily experiences of countless individuals residing in major cities. Its pivotal role extends beyond mere convenience, as transportation systems significantly shape energy consumption patterns and substantially impact the environment. Our choices in optimising transportation affect the efficiency of our daily commutes and play a critical role in determining the sustainability of our cities and the planet's well-being. As cities grow and face escalating congestion, energy usage, and environmental sustainability challenges, exploring innovative solutions becomes imperative.

Within this context, the convergence of quantum computing and transportation optimisation stands out as a compelling pathway toward minimising commuting times, energy consumption, and carbon emissions and enhancing the efficient utilisation of vehicles. In a hypothetical urban environment without private vehicles, the focus lies in designing a quantum algorithm capable of optimising public transportation systems to offer citizens seamless, eco-friendly, and energy-efficient travel experiences. Additionally, exploration extends to assessing the viability of integrating such a system with vehicles owned by external entities.

Building upon prior research that explores the quantum iteration of the capacitated vehicle routing problem, the objective is to devise an algorithm adept at dynamically allocating resources, such as large buses and small cars, in response to real-time demand and passenger distribution across geographical locations. Notably, existing studies in this realm indicate progress, yet they underscore the persistent limitations, leaving considerable scope for further advancements and refinements.

We intend to use the Qiskit framework, a robust quantum computing platform, to implement an algorithm to optimise public transportation. We want to simulate real-world complexities by employing mock data representative of a major city's public transport system. Furthermore, we intend to enhance authenticity by exploring the integration of actual data from a major city. This approach aims to validate the algorithm's efficacy and demonstrates its relevance to the intricacies of urban mobility.

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Abbreviations and Symbols

CVRP	Capacitated Vehicle Routing Problem
HQEA	Hybrid Quantum Evolution Algorithm
IQEA	Improved Quantum Evolution Algorithm
KP	Knapsack Problem
NISQ	Noisy Intermediate-Scale Quantum
NP	Nondeterministic Polynomial Time
PSO	Particle Swarm Optimization
QC	Quantum Computing
QAOA	Quantum Approximate Optimization Algorithm
QEA	Quantum Evolution Algorithm
QPU	Quantum Processing Unit
QUBO	Quadratic Unconstrained Binary Optimization
Qubit	Quantum Bit
TSP	Traveling Salesman Problem
VNS	Variable Neighborhood Search

Chapter 1

State of the Art

1.1 Introduction

This chapter aims to present a thorough and contemporary understanding of the theme explored in this dissertation. It is organized into two main sections.

The first one, Background, is structured into distinct topics, providing insights into the key concepts of the dissertation's theme. Specifically, it is divided as follows:

- **Urban Transportation**: Explores the functioning of contemporary urban transportation in major cities and outlines existing challenges in these systems. Then, it explains the capacitated vehicle routing problem and how it can be applied to the topic.
- **Quantum Computing**: Describes the principles of quantum computing, its operational mechanisms, advantages over classical computers, and exploration of hybrid systems.
- **Quantum Hardware**: Discusses the current state of hardware for quantum computers in the NISQ era, available technologies, and their limitations.
- **Quantum Algorithms**: Explores established quantum algorithms tailored for addressing the intricacies of transportation system optimization, mainly focusing on the Capacitated Vehicle Routing Problem (CVRP).

The second section, Related Work, examines current methodologies addressing the issues outlined in the dissertation. This analysis is grounded in recent papers published over the past few years.

1.2 Background

1.2.1 Urban Transportation

Urban transportation in major cities is a multifaceted system that involves a combination of private cars, public transport and pickup services provided by modern smartphone applications, influencing the daily experiences of countless individuals. The intricate interplay of these transportation mechanisms significantly shapes energy consumption patterns and has substantial environmental implications. As cities grapple with congestion, energy usage, and environmental sustainability challenges, exploring innovative solutions becomes increasingly imperative.

In this dissertation, the primary focus is exclusively on optimising public transport within urban environments. The envisioned system accommodates various public vehicles, including small cars and buses of varying sizes. Furthermore, it aims to provide a seamless and eco-friendly travel experience by allowing for pickups anywhere within a designated area or city, capable of competing with the current options.

Therefore, the problem at the core of this research aligns with the **capacitated vehicle routing problem (CVRP)**, a well-established optimisation challenge in the field of transportation. The CVRP involves efficiently allocating resources, in this case, public vehicles with different capacities, to pick up passengers from diverse locations within a given area. While the primary objective is to minimise commuting times, the optimisation extends to encompass considerations of energy consumption and carbon emissions.

As a natural extension of the CVRP, it is possible to add pickup time as a potential constraint within the optimisation problem, creating variations of the initial problem (as shown in figure 1.1). This addition further refines the algorithm's ability to dynamically allocate resources in response to real-time demand and passenger distribution across geographical locations.

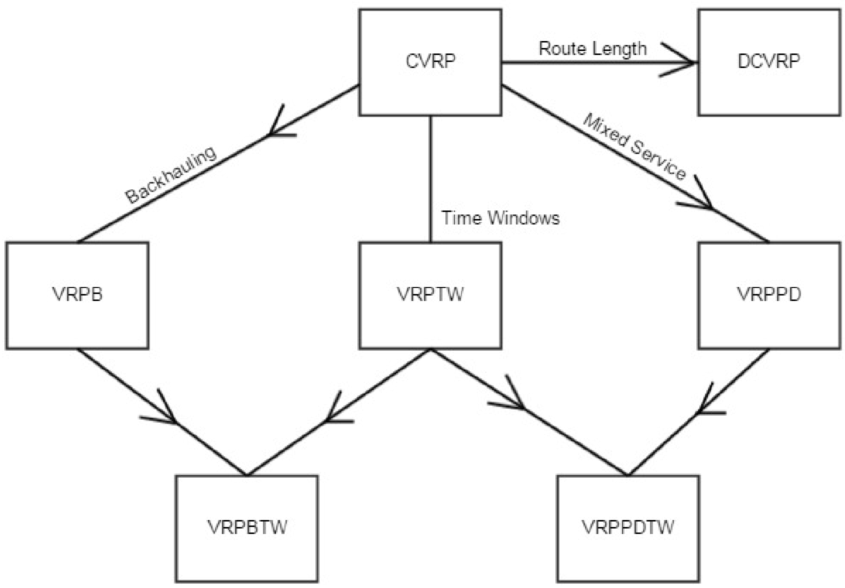

Figure 1.1: Variations of the Capacitated Vehicle Routing Problem [13]

1.2.1.1 Capacitated Vehicle Routing Problem

The Capacitated Vehicle Routing Problem (CVRP) involves the deployment of a fleet of vehicles, each subject to capacity constraints, to collect goods or passengers from diverse locations. The challenge inherent in CVRP lies in identifying the most optimal set of routes for these vehicles to achieve an objective function, as shown in figure 1.2, often focused on optimizing factors such as travel time. Due to its NP-hard nature, finding the globally optimal solution with classical algorithms is considered inefficient, making the quest for high-quality approximate solutions complex and demanding [3].

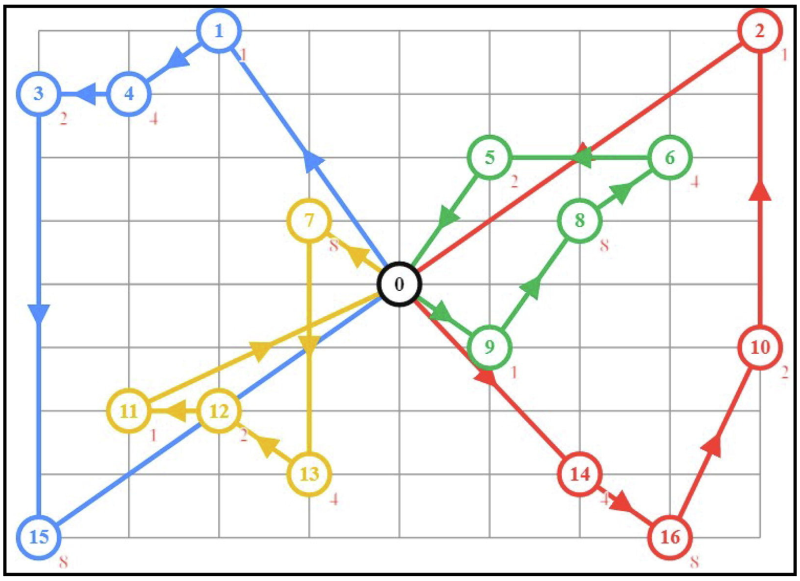

Figure 1.2: Example of an output of the CVRP [27]

The CVRP encompasses both the Bin Packing Problem and the Traveling Salesman Problem (TSP) as specific instances, representing a conceptual convergence of these well-studied problems. The integer programming formulation of this routing model introduces capacity constraints that serve as the crucial link connecting the fundamental routing and packing structures underlying the problem [25].

Potential solutions to the Traveling Salesman Problem (TSP) can be conceptualized as permutations of nodes representing the visit order. This problem can be formulated by introducing variables denoting a specific node i and its location j in the visit cycle. The cost of traversing the route based on edges can be expressed as:

$$c(x) = \sum_{u,v} W_{u,v} \sum_{j} x_{u,j} x_{v,j+1} \tag{1.1}$$

Here, $W_{u,v}$ represents the edge cost from node u to node v, and the decision variable $x_{u,j}$ equals 1 if node u has been visited at position j, and 0 otherwise [15]. The optimization task involves minimizing the aforementioned cost function while adhering to specific constraints. These constraints ensure that each node appears once in the visit cycle, and each visit-cycle position is utilized once.

The CVRP can be viewed as an extension of the TSP to incorporate multiple vehicles, each subjected to an associated capacity constraint that imposes an upper limit on the number of nodes it can visit. A straightforward extension of the previous formulation involves introducing an additional *vehicle* index to each decision variable: $x_{i,j,v}$ is set to 1 if and only if node i is visited at position j by vehicle v. The availability of space on the vehicle for passengers or goods will determine the value of this index.

While exact solutions for CVRP can be obtained through advanced solvers for problem sizes of up to approximately 150 passenger locations with multiple vehicles, execution times may become impractical depending on the problem specifications (e.g., 11 days for a 284-node problem). The most effective heuristic solutions consistently yield solutions within 1%

In addition to its applications in transportation optimization, the CVRP finds utility in various contexts, including first-mile/last-mile services, emergency evacuation procedures, and shipment services. The versatility of the CVRP extends its relevance beyond conventional transportation scenarios, making it a valuable tool in addressing diverse logistical challenges.

1.2.2 Quantum Computing

Quantum computing represents a novel paradigm in computation, drawing on the principles of quantum mechanics. Unlike classical computing, which relies on bits as binary units, quantum computers utilize qubits that are capable of existing in multiple states simultaneously. This unique property, known as superposition, enables quantum computers to conduct parallel computations. Additionally, the phenomenon of entanglement allows qubits to be interconnected, facilitating more efficient problem-solving. This section provides an in-depth exploration of quantum computing, clarifying its essential attributes, potential applications, and inherent limitations.

1.2.2.1 Quantum Bits

A quantum bit, or qubit, is a fundamental unit of information in quantum computing. It is depicted as a unit vector within a two-dimensional complex vector space, with a specific basis denoted by $\{|0\rangle, |1\rangle\}$. In the domain of quantum computation, the basis states $|0\rangle$ and $|1\rangle$ are utilized to represent classical bit values 0 and 1, respectively [6]. Nevertheless, quantum bits can also be expressed in an alternative arbitrary basis, for example, $\{|+\rangle, |-\rangle\}$.

The qubit's basis representation relies on the **bracket notation**, a concept introduced by Dirac for expressing a Hilbert space vector in quantum mechanics [5]. Alternatively, the basis can be conveyed in matrix form:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{1.2}$$

1.2.2.2 Superposition

In contrast to classical bits, which can only be in states 0 or 1, qubits have the unique ability to exist in a superposition of $|0\rangle$ and $|1\rangle$. This characteristic enables qubits to occupy multiple states concurrently, represented as a linear combination of all possible states.

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \equiv \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} \equiv \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \tag{1.3}$$

where α and β are complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$ [6]. Intuitively, α^2 and β^2 denote the probabilities of the quantum position being in that state after measurement, as further explained in section 1.2.2.4. It is important to note that superposition is basis-dependent, signifying that a qubit may exist in a superposition state on one basis but not in another [7].

As only two numbers are required to represent a qubit, it can be mapped onto an arrow originating from the origin and extending to the three-dimensional sphere in $\mathbb{R}^3$ with a radius of 1, commonly referred to as the **Bloch sphere**. Each qubit can be depicted using two angles that define the orientation of this arrow, as shown in figure 1.3.

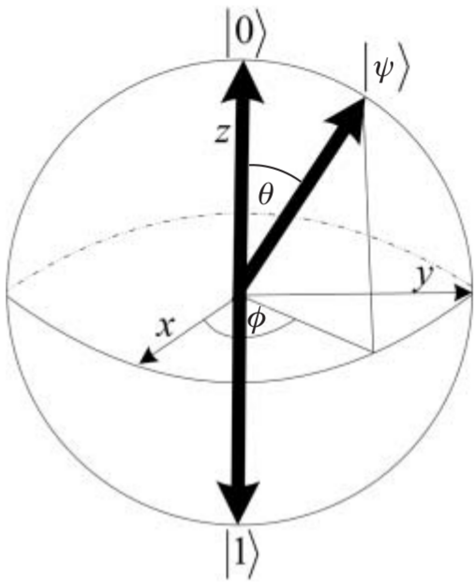

Figure 1.3: Bloch sphere representation [19]

where $0 \leq \phi < 2\pi$ and $0 \leq \theta < \frac{\pi}{2}$. That said, the superposition can be written as shown in equation 1.2.2.2 [28].

$$|\psi\rangle = cos\frac{\theta}{2}\,|0\rangle + e^{i\phi} sin\frac{\theta}{2}\,|1\rangle \tag{1.4}$$

1.2.2.3 Multi-qubit States

A system comprising n qubits can exist in a superposition of all 2^n possible states, demonstrating the true potential of quantum computation [6]. Consider a system with two qubits, where there are four possible states: $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$, similar to a classical computer. However, in quantum systems, the state can be a superposition of all these possibilities:

$$|\psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma|10\rangle + \sigma\,|11\rangle \tag{1.5}$$

Here, α, β, γ, and σ are complex numbers, and the sum of their squares equals 1. Mathematically, a basis state with n qubits is expressed as the tensor product of its individual qubits:

$$\{|0\rangle \otimes |0\rangle\,, |0\rangle \otimes |1\rangle\,, |1\rangle \otimes |0\rangle\,, |1\rangle \otimes |1\rangle\} = \{|00\rangle\,, |01\rangle\,, |10\rangle\,, |11\rangle\} \tag{1.6}$$

1.2.2.4 Measurement

In quantum computing, the measurement process stands out as a particularly counter-intuitive aspect. In contrast to classical computers, wherein the state of a system can be repeatedly determined at will, quantum systems, particularly qubits, only allow the determination of a single characteristic at a time. For instance, it is feasible to ascertain whether the system is in the state $|0\rangle$ or $|1\rangle$, but this measurement is inherently random and alters the system's state [28].

In the measurement process, the likelihood of the system being in a given state corresponds to the square of the respective coefficients, as shown in equation 1.2.2.2. The measurement of systems comprising multiple qubits can be approached by conducting a sequence of individual bit measurements within the chosen basis [6]. The outcome can then be stored in a classical register.

From a mathematical perspective, the measurement process is described by the observable $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ [28]. An observable represents a measurable physical quantity defined by a Hermitian operator A acting on Hilbert space ($A^\dagger = A$) [29]. The potential outcomes of the measurement correspond to the eigenvalues of the state's matrix.

The measurement outcome depends on the selected basis, and the result will vary accordingly. While conducting measurements on an arbitrary orthonormal basis is possible, only one basis can be employed. This limitation arises due to the destruction of the initial superposition state following the measurement, a characteristic sharply contrasting with the behaviour of classical systems.

1.2.2.5 Quantum Gates

We have observed quantum states that undergo change solely upon measurement. Nevertheless, the most valuable aspect of a quantum system lies in its ability to undergo dynamic changes prior to measurement, facilitated by the application of **quantum gates**. In mathematical terms, quantum gates are linear transformations that maintain orthogonality, referred to as **unitary** transformations. These transformations can be represented by unitary matrices whose conjugate transpose is equal to themselves ($U^\dagger U = I$). Unitary transformations can also be conceptualized as rotations within a complex vector space. A crucial implication of these transformations is their reversibility; hence, quantum gates must inherently be reversible [6].

Quantum gates perform operations analogous to classical logical gates, such as AND, OR, XOR, and NOT. In this context, the input and output of the gates are quantum states, and they

Gate	Description	Matrix
Identity (I)	Simplest gate, does not alter the state. Can be adapted to multiple qubits.	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
Hadamard (H)	Creates an equal superposition when given a basis state (e.g. $\|0\rangle$).	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Pauli-X (X)	Quantum equivalent of the NOT classical gate for the basis $\{\|0\rangle, \|1\rangle\}$. When applied, rotates the x axis of the Bloch sphere by π radians	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	When applied, rotates the y axis of the Bloch sphere by π radians	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	When applied, rotates the z axis of the Bloch sphere by π radians. Leaves the basis state $\|0\rangle$ and maps $\|1\rangle$ to $-\|1\rangle$, thus being also called phase-flip.	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Phase (S, P)	Family of single-qubit gates that leave the basis state $\|0\rangle$ and map $\|1\rangle$ to $e^{i\phi}\|1\rangle$. The probability of measurement is unchanged after this gate, but the phase of the state is modified.	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$
CNOT	Applies the X gate on the second qubit if the first one is $\|1\rangle$. Otherwise, both are unchanged.	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
SWAP	Swaps two qubits, with respect to the $\{\|0\rangle, \|1\rangle\}$ basis.	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Table 1.1: Most common quantum gates

are characterized by matrices of dimensions 2^k, where k denotes the number of qubits in the state. While quantum gates can be constructed arbitrarily, a standard set of gates is commonly employed, particularly those detailed in table 1.1, which operate on either 1 or 2 qubits [18].

1.2.2.6 Quantum Circuits

Quantum circuits are employed to visually depict a sequence of quantum gates and measurements applied to qubits. These circuits serve as a model of quantum computation based on classical circuits. Each qubit has its quantum wire, upon which corresponding quantum gates are applied. Additionally, a wire is commonly used to denote the classical register for storing measurement values. An illustrative example is presented in figure 1.4.

Quantum circuits should be interpreted chronologically from left to right. The vertical axis corresponds to the qubits, with their order subject to variation in different implementations. In this context, the top qubit is considered the most significant. Multi-qubit gates are typically defined by connecting the relevant qubits with a vertical line.

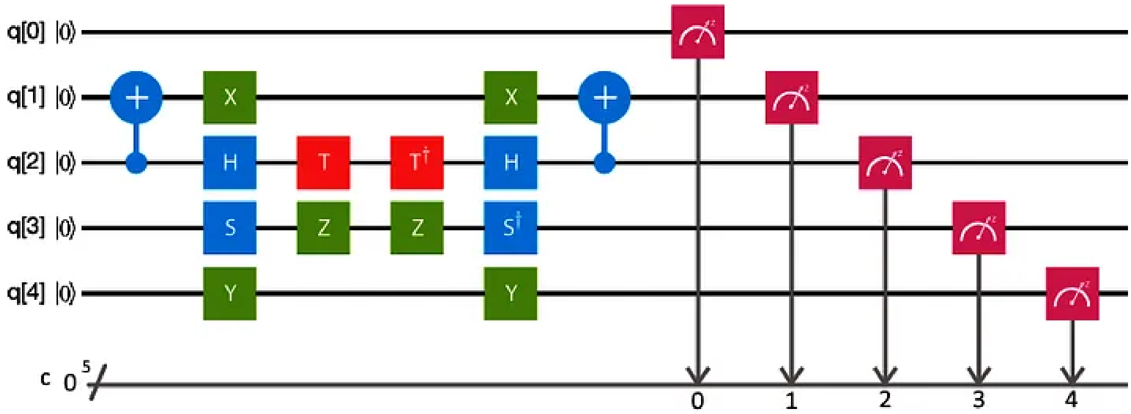

Figure 1.4: Example of a quantum circuit [23]

1.2.2.7 Entanglement

Quantum entanglement is a physical phenomenon manifested when multiple qubits exhibit correlated states. The implications of entanglement suggest the potential for quantum computers to outperform classical computers, achieving notable speedup. Through entanglement, qubits become correlated, revealing hidden information. This property is a crucial advantage in quantum computing and is harnessed by numerous algorithms [4].

In intuitive terms, if one qubit's measurement influences the measurement of another, then they are considered entangled [6]. A straightforward illustration of this phenomenon is the following state, recognized as one of the *Bell* states:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{1.7}$$

In this scenario, measuring one of the qubits immediately discloses the state of the other, even without directly measuring it. Before any measurement, the probabilities of both qubits being in states $|0\rangle$ or $|1\rangle$ are each 50%. If, for instance, the first qubit is measured and found in the state $|0\rangle$, then the second qubit is guaranteed to be in the state $|0\rangle$ with 100% probability. This highlights the concept that entanglement unveils concealed information, a capability beyond the reach of classical computers.

From a mathematical perspective, a multi-qubit state is deemed entangled if it cannot be represented as a product state, i.e., it is not separable. A separable state can be expressed as a tensor product of basis states:

$$|\psi_{\text{separable}}\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \tag{1.8}$$

Nevertheless, establishing whether a general multi-qubit state can be expressed as a product state can be challenging. A more straightforward test for entanglement involves checking whether measuring one qubit alters the probability distribution of the second qubit. If the test is affirmative, the system is considered entangled. However, a negative result does not necessarily rule out entanglement, as hidden information might be associated with the coefficients' signs, which do not impact the probability distribution [4].

Creating entanglement between two qubits can be achieved quite straightforwardly. A simple method involves applying a Hadamard gate to the first qubit and subsequently applying a CNOT gate between the first and second qubits. This procedure generates the previously mentioned *Bell* state, as depicted in the circuit illustrated in figure 1.5.

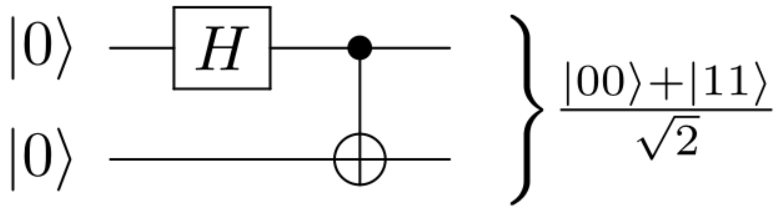

Figure 1.5: Quantum circuit generating an entangled state [9]

Including the previously provided example, four *Bell* states hold fundamental significance in quantum computing. These states are crucial as they represent the most straightforward instances of entanglement and play a key role in essential algorithms such as quantum teleportation and superdense coding [7]:

$$
\begin{aligned}
|\Phi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\
|\Phi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\
|\Psi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\
|\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)
\end{aligned}
\tag{1.9}
$$

1.2.2.8 Why use Quantum Computing?

As explained earlier, the power of quantum computation lies in the non-classical encoding of information in qubits, allowing computations to harness quantum effects like entanglement that are not accessible in classical computing [22]. Numerous algorithms leverage these effects; however, quantum computers are not intended to replace classical counterparts. Instead, quantum computation aims to complement classical computing, addressing tasks that are inherently inefficient for classical systems or enhancing the efficiency of existing operations. Consequently, hybrid systems, integrating classical and quantum components, have gained prominence. This approach allows real-world applications to capitalize on the strengths of each paradigm, employing quantum algorithms when they provide a speedup over classical counterparts (quantum advantage).

In Section 1.2.4, we explore examples of prominent algorithms pertinent to transport optimization. Additionally, Section 1.3 delves into current applications within the broader context of related work.

1.2.3 Quantum Hardware

Quantum hardware is currently in the Noisy Intermediate-Scale Quantum (NISQ) era and is anticipated to remain in this phase in the near future. While quantum computers with 50-100 qubits may outperform today's classical digital computers in specific tasks, noise in quantum gates limits the reliable execution of larger quantum circuits. Although NISQ devices hold significant value for research purposes, a 100-qubit quantum computer will not immediately revolutionize the world [20].

In the short term, quantum computers will probably serve as specialized tools, with users accessing them predominantly through the cloud for research purposes or to attain some speedup. Presently, IBM provides quantum computers featuring 127 qubits, and their roadmap outlines projections of reaching up to 1000 qubits in the coming years, though this remains uncertain.

While achieving quantum computers with more than 100 qubits represents a noteworthy milestone in quantum technology, it is noteworthy that a 2000-qubit quantum device, the D-Wave 2000Q machine, has been available since 2017. However, it is crucial to recognize that this machine operates as a quantum annealer rather than a circuit-based quantum computer. It effectively addresses optimization problems through a different approach than the execution of a quantum circuit. Presently, no compelling theoretical argument or conclusive experimental evidence demonstrates that quantum annealers can significantly accelerate the time to solution compared to the most advanced classical hardware [20].

For a fault-tolerant quantum computer, surpassing the limitations of NISQ, to be viable, it must satisfy the following five criteria. Although these criteria have yet to be fully met, they serve as guiding principles to enhance and refine quantum hardware progressively over time [11].

1. A scalable physical system containing well-defined qubits.
2. Capability for deterministic initialization of the system into a well-defined initial state.
3. Availability of a set of universal quantum gates, including single-qubit and entangling two-qubit gates.
4. Qubit decoherence times significantly exceeding gate times.
5. Capability to perform measurements on the qubit state with high accuracy.

1.2.4 Quantum Algorithms

This section delves into well-known quantum algorithms designed to navigate the complexities of transportation system optimization. Grounded in the principles of quantum computing, these algorithms present innovative solutions for addressing challenges associated with the Capacitated Vehicle Routing Problem and related optimization tasks.

1.2.4.1 Quadratic Unconstrained Binary Optimization

The Quadratic Unconstrained Binary Optimization (QUBO) model is a mathematical formulation for solving quadratic combinatorial optimization problems. It involves finding the optimal configuration of binary variables to minimize or maximize a quadratic objective function, subject to certain constraints. In simpler terms, it is a way to represent and solve optimization problems where the goal is to make binary choices that lead to the best overall outcome based on a quadratic function [18].

The QUBO model has effectively addressed significant optimization challenges, including multiple knapsack problems, clique problems, graph colouring, and warehouse location problems [8].

A **formal formulation** of the QUBO model is presented as the optimization problem:

$$\text{minimize/maximize } y = x^T Qx, \quad x \in \{0,1\}^n \tag{1.10}$$

where x is a vector of binary decision variables and Q is a square matrix of constants. The Q matrix is commonly assumed to be symmetric or in upper triangular form, depending on the framework implementing the model [8].

The pure form of the QUBO model lacks constraints, which poses a challenge when dealing with problems involving real-world constraints. Many practical scenarios need additional conditions to be met during the optimization process. To address this, **quadratic penalties** are introduced into the objective function as an alternative to explicitly enforcing classical constraints. These penalties are structured to be zero for feasible solutions and assume a considerably significant value for infeasible solutions. Examples of such penalties for commonly encountered constraints are outlined in Table 1.2 [8].

Classical Constraint	QUBO Penalty
$x+y \leq 1$	$P(xy)$
$x+y \geq 1$	$P(1-x-y+xy)$
$x+y=1$	$P(1-x-y+2xy)$
$x \leq y$	$P(x-xy)$
$x_1+x_2+x_3 \leq 1$	$P(x_1x_2+x_1x_3+x_2x_3)$
$x=y$	$P(x+y-2xy)$

Table 1.2: Table of a few known constrain/penalty pairs [8]

To illustrate the idea, consider a problem of the form $Min\ y = f(x)$ subject to the constraint $x_1+x_2 \leq 1$, where x_1 and x_2 are binary variables. As long as $f(x)$ is linear or quadratic, then this will be the QUBO form of the problem: *minimize* $y = f(x) + P(x_1x_2)$.

Quantum Approximate Optimization Algorithm

The QUBO framework offers a convenient embedding for NP optimization problems and shares a strong relationship with the quantum Ising model. This alignment makes QUBO formulations seamlessly compatible with the Quantum Approximate Optimization Algorithm (QAOA). Within the QAOA framework, QUBO problems find efficient representation, where each binary optimization variable corresponds to a single qubit [3].

Operating within a hybrid algorithmic framework that combines classical and quantum computing components, as shown in figure 1.6, QAOA employs a quantum circuit consisting of two interleaved modules:

- A problem or cost unitary, which applies a phase shift to solutions proportional to their quality.
- A mixer unitary, which mixes quantum amplitudes between solutions to explore the search space.

A classical optimization loop iteratively adjusts the parameterized modules, ensuring that the combined effects of exploration and quality-dependent phase shifts enhance the likelihood of measuring high-quality outputs. The quantum circuit undergoes multiple runs to generate a set of measured states (candidate solutions). The classical optimizer refines the variational quantum circuit parameters until convergence or a predefined stopping condition is met. Ultimately, the algorithm returns the best-obtained candidate solution [3].

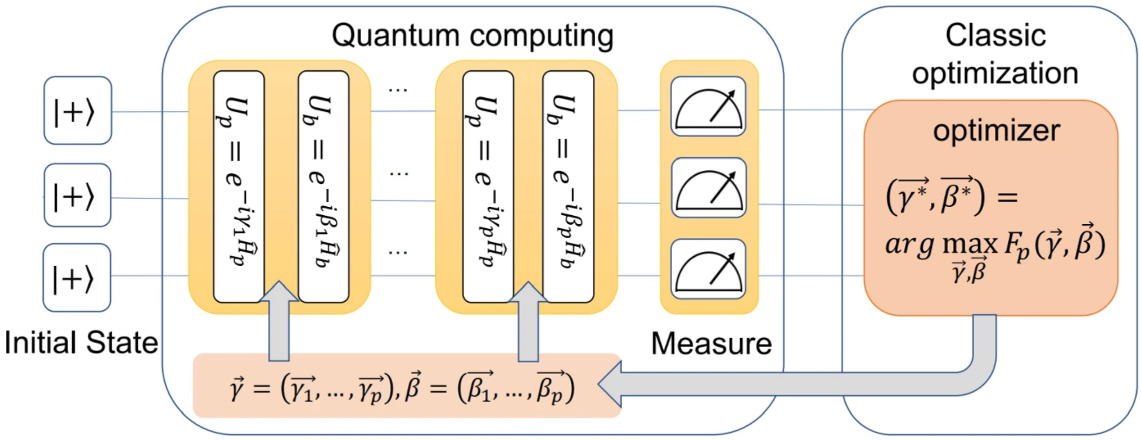

Figure 1.6: Diagram showing the principles of QAOA [2]

1.2.4.2 Quantum Annealing

Quantum annealing is a metaheuristic designed for solving intricate optimisation problems akin to simulated annealing in classical computing. D-Wave's quantum annealing algorithm is implemented in hardware, employing a framework of analogue control devices to manipulate a set of qubits based on a time-dependent Hamiltonian, $H(t)$, as illustrated in Equation 1.2.4.2 [24].

$$H(t) = s(t)H_I + (1 - s(t))H_P \tag{1.11}$$

The fundamental concept of quantum annealing involves a physical interpolation between an initial Hamiltonian H_I and a problem Hamiltonian H_P corresponding to the optimal solution of the specified problem. This interpolation follows an adiabatic evolution path mathematically represented by the function $s(t)$, decreasing from 1 to 0. If this transition is executed sufficiently slowly, the probability of finding the ground state of the problem Hamiltonian approaches 1 [24].

Any optimisation problem formulated as a QUBO can be addressed using quantum annealing. In such instances, the Hamiltonian corresponds to the minimised or maximised function, represented as $x^T Qx$ [21]. Constraints can be incorporated in the same manner as the explanation in section 1.2.4.1.

1.2.4.3 Quantum Evolution Algorithm

The Quantum Evolution Algorithm (QEA) is a probabilistic algorithm that incorporates certain characteristics of classical evolutionary algorithms, including representing individuals, fitness functions, updating processes, and mutations [14]. The QEA procedure is outlined as follows [10]:

1. Randomly generate an initial population $P(t) = \{p_1^t, \ldots, p_n^t\}$, where t is the generation number (0 in this case), and $p_i^t = \begin{bmatrix} \alpha_1^t & \ldots & \alpha_m^t \\ \beta^t & \ldots & \beta^t \end{bmatrix}$, given m qubits.

2. Form a binary population $R(t) = \{r_1^t, \ldots, r_n^t\}$ by observing the states of $P(t)$ at generation t. Each binary solution is a binary string of length m, created by selecting either 1 or 0 for each bit using the probability of the qubits.

3. Evaluate each solution in $R(t)$ and record the best solution. If the stopping condition is met, output the best solution; otherwise, proceed to the next steps.

4. Apply a rotation gate $U(\theta)$ to update $P(t)$.

5. Set $t = t + 1$ and return to step 2.

Several algorithms may implement specific steps on a classical computer, leading to the realisation of a hybrid algorithm known as the Hybrid Quantum Evolution Algorithm (HQEA). Other researchers have focused on enhancing the Quantum Evolution Algorithm (QEA), involving tasks such as redesigning the encoding mechanism, optimising rotation angles, and appropriately defining rotation directions. These improved versions are commonly referred to as Improved Quantum Evolution Algorithms (IQEA) [14].

1.3 Related Work

This section explores the current literature on the Capacitated Vehicle Routing Problem (CVRP), specifically emphasizing implementations utilizing quantum computing. The first part delves into existing CVRP implementations using classical computing. Subsequently, the second part introduces various quantum approaches, along with the outcomes already achieved or anticipated in the near future, considering the constraints of the currently limited quantum hardware.

1.3.1 Classical Approaches

The Vehicle Routing Problem (VRP) and its various variants represent longstanding challenges within the NP group, leading to an extensive exploration of solutions and proposals. Praveen et al. conducted a survey on research papers related to the CVRP [27]. This section will be grounded in the key solutions highlighted by their comprehensive survey.

In 2017, Ali Asghar Rahmani Hosseinabadi et al. [1] developed the CVRP_GELS algorithm based on criteria used in physics concerning searching and random search. The defined method works well when the problem size is more significant and achieves less compute time than the state-of-the-art, except for a few instances.

In 2017, M.A. Hannan et al. [17] devised a route optimization solution for waste pickup using a modified version of Particle Swarm Optimization (PSO). While the results were positive, the approach's feasibility for real-world scenarios remains to be validated, suggesting the potential for future work to involve the development of smart bins.

In 2017, Kangzhou Wanga et al. [12] employed integer programming and Variable Neighborhood Search (VNS) algorithms to address the CVRP. Their approach resulted in a significant reduction in both the number of required drivers and fuel costs.

In 2018, Mario Marinelli et al. [16] successfully employed a Fuzzy C-means approach to cluster end users to streamline civic carriage distribution in urban logistics. This innovative approach contributes to developing green routing strategies, primarily enhancing traffic flow and reducing discharge costs.

In 2018, Valeria Leggieri et al. [26] introduced metaheuristics comprising three linear stages. Initially, the problem size is significantly reduced by eliminating unwanted arcs, followed by deriving a reasonable solution. Finally, the optimal solution is generated. The study suggests that defining improved formulations can alleviate the computational burden, emphasizing the need for future research to develop faster approaches for obtaining initial solutions.

1.3.2 Quantum Approaches

1.3.2.1 QAOA Implementation

Bentley et al. [3] developed a framework to achieve potential performance enhancement through quantum algorithms tailored for transport optimization, explicitly addressing the Capacitated Vehicle Routing Problem (CVRP).

In their approach, the Quantum Approximate Optimization Algorithm (QAOA) model is employed to leverage a hybrid system comprising classical and quantum components. The authors introduced an innovative binary method for encoding the CVRP for quantum algorithms, thereby reducing the qubit resource requirements. This method, initially applied to the problem of clique partitioning, was extended from a representation of the Traveling Salesperson Problem (TSP) by incorporating an additional constraint related to the capacity of each vehicle into each decision variable for the CVRP.

Apart from the high-level algorithm, the authors introduced two advancements to improve the circuit's success on small-scale quantum computers. Firstly, they incorporated a hard mixer designed to limit the algorithm's exploration to the valid solution space, in contrast to the conventional Quadratic Unconstrained Binary Optimization (QUBO) approach, where penalties are added to discourage invalid solutions. Secondly, they utilized Q-CTRL's Fire Opal software for efficient hardware-aware implementation. To illustrate, they applied a circuit for routing a vehicle between a depot and two passenger nodes, which involved four two-qubit gates.

The authors showcased over 20X error reduction in their example compared to the standard QAOA implementation despite employing a smaller but non-scalable circuit. According to their solution, addressing a problem involving seven vehicles with a maximum capacity of 20 passengers needs approximately 1000 qubits, a demand exceeding the capabilities of current hardware (with 127-qubit devices currently available). However, this capacity aligns with IBM's quantum systems roadmap, indicating a potential feasibility in the near future.

1.3.2.2 Quantum Annealing Implementation

Feld et al. [24] and Harikrishnakumar et al. [21] both describe implementations of the CVRP on a quantum annealer using a QUBO formulation with considerably different approaches.

Feld introduces three approaches (both quantum and hybrid) based on two algorithmic phases. The initial phase involves a clustering process using the Knapsack Problem (KP), followed by a routing phase utilizing the Travelling Salesman Problem (TSP). Figure 1.7 illustrates the three approaches. In the experiments, the hybrid approach proved to be the most effective, while the first two approaches represented variations of a fully quantum algorithm, incorporating one or two QUBO matrices.

Given the limited qubit availability on the D-Wave Quantum Processing Unit (QPU), the hybrid solution method outlined in the study has yet to yield evident advantages in solution quality or computational time. However, the authors have introduced an approach to partition complex combined problems and address them through a hybrid approach employing a quantum annealer. This methodology serves as a foundation for future research, anticipating improvements in hardware capacity [24].

On the other hand, Harikrishnakumar formulates the problem by defining an objective function that minimizes the distance travelled by all vehicles, along with a set of constraints. Subsequently, these components are translated into Hamiltonian terms and combined to create the overall Hamiltonian, as shown in Equation 1.3.2.2. In this equation, each term signifies the summation of the objective function (H_0) and individual constraints (H_{C_i}) [21].

$$H_F = H_0 + \sum_{i=8}^{8} H_{C_i} \tag{1.12}$$

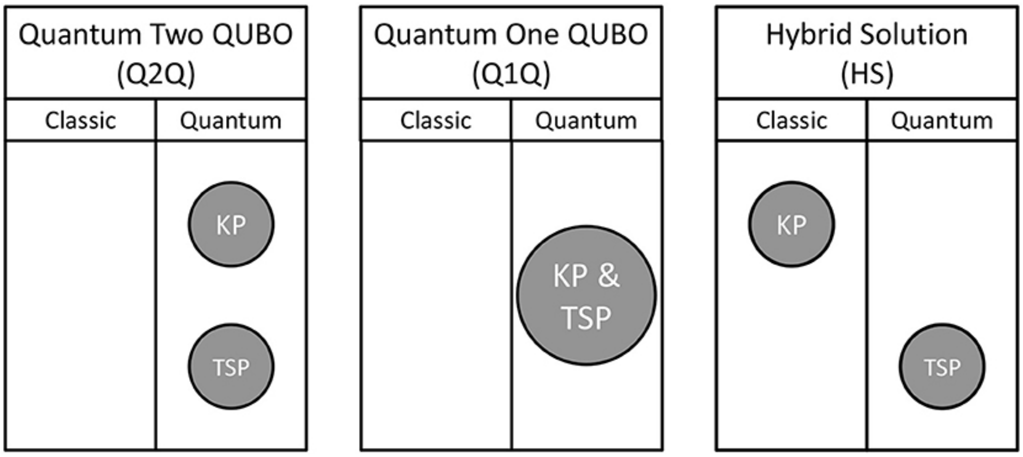

Figure 1.7: Assignment of the clustering and routing phases in 3 different approaches

This study acknowledges the potential implementation of the described approach on the D-Wave 2000Q (a machine with 2048 qubits) but has yet to be executed, leaving this task for future research. Consequently, no specific results from this implementation were presented.

1.3.2.3 Quantum Evolution Algorithm Implementation

Cui et al. [14] propose a novel Improved Quantum Evolution Algorithm (IQEA) with a mixed local search procedure for addressing the Capacitated Vehicle Routing Problem (CVRP). Despite the study's 2013 timestamp, their approach remains relevant in this literature review. Initially, an IQEA is constructed, incorporating a double-chain quantum chromosome, new quantum rotation schemes, and a self-adaptive quantum NOT gate to initialize and generate feasible solutions. To enhance the searching capability of IQEA, three local search procedures are integrated into a consolidated local search mechanism:

- **1-1 exchange:** Attempts to interchange one client from one route with another client in a different route when the distance between the two clients is below a predetermined threshold.
- **1-0 exchange:** Removes a client from the first route and inserts it into another route.
- **2-OPT:** Exchanges the visiting sequences of two different clients within the same route.

The final local search algorithm executes each of these steps conditionally for a predefined number of times, resulting in improved performance compared to using each method individually. The algorithm is named IQEA+, and the pseudocode can be seen in figure 1.8.

The experiments conducted in the study reveal that the proposed IQEA+ shows potential in addressing the Capacitated Vehicle Routing Problem (CVRP) to a certain extent, achieving relatively high precision and speed. However, the findings also indicate that while IQEA+ excels in

```
for i = 1 to K do
  Randomly select 2 candidate routes;
  Calculate the actual carrying capacity (AC) of each vehicle.
  if AC < Burden Rating (BR) then
    Run 1-1 exchange and 1-0 exchange 5 times.
    if solutions improved and constraints meet then
      Run 2-OPT 5 times
    else
      Roll back to other routes
    end if
  else
    Run 1-1 exchange and 1-0 exchange 5 times.
    while solutions improved do
      Run 2-OPT 5 times
    end while
  end if
end for
```

Figure 1.8: Pseudoce of the IQEA+ algorithm [14]

searching precision compared to other classical algorithms, it falls short in efficiency. Notably, the local search procedures consume more than half of the total computing time, particularly as the scale of the problem increases.

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