ENHANCED QUANTUM ANNEALING TSP SOLVER (EQATS): ADVANCEMENTS IN SOLVING THE TRAVELING SALESMAN PROBLEM USING D-WAVE'S QUANTUM ANNEALER

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ABSTRACT

In this paper, we examine the use of quantum annealing for the Traveling Salesman Problem (TSP) using the D-Wave Advantage quantum annealer and its "Pegasus" architecture. We introduce a refined Quadratic Unconstrained Binary Optimization (QUBO) formulation that simplifies the problem by eliminating the first node and reallocating its effect, thereby reducing qubit requirements and improving efficiency. We formulate the TSP as a QUBO problem and compare quantum solutions with classical solutions for instances involving 8, 9, and 10 cities. Additionally, we compare our solver with the D-Wave TSP solver for the 20-city case. Our proposed method outperforms the D-Wave solver and achieves nearly optimal solutions. Thus, our key contribution is a critical analysis of quantum annealing's performance and proposed enhancements to address existing limitations. This research provides insights into the strengths and weaknesses of modern quantum techniques and offers guidance for future advancements in quantum optimization.

1 INTRODUCTION

In computational complexity theory, the distinction between $\boldsymbol{P}$ and $\boldsymbol{NP}$ is fundamental. Class $\boldsymbol{P}$ consists of decision problems that can be solved in polynomial time by a deterministic Turing machine. Conversely, $\boldsymbol{NP}$ consists of decision problems for which a given solution can be verified in polynomial time by a deterministic Turing machine. NP-hard problems are those as difficult as the hardest problems in $\boldsymbol{NP}$. Despite extensive research and significant progress in understanding the nature of these problems, the question of whether $\boldsymbol{P} = \boldsymbol{NP}$ remains one of the most important open challenges in computer science. The consensus among most researchers tends to lean towards the belief that $\boldsymbol{P} \neq \boldsymbol{NP}$, though a formal proof has yet to be discovered Cook (2000); Aaronson (2016); Sudan (2010); Wigderson (2019). The resolution of this problem holds profound implications for both theoretical computer science and practical applications across various fields. This classification underscores the theoretical and practical importance of NP-hard problems, given their prevalence in real-world scenarios such as cryptography, resource allocation, and optimization problems where efficient solutions are critical yet elusive due to computational constraints. Castaneda et al. (2022); Juan et al. (2018); Tindell et al. (1992); Haider et al. (2009); Alber (2003); Lanza-Gutierrez et al. (2011); Zhao et al. (2021); Erwin & Engelbrecht (2023); Giannakouris et al. (2010); Nikoloski et al. (2008); Nagarajan & Pop (2009); He et al. (2010); Ilango et al. (2020); Ning (1994).

Hence, we are in the context of $\boldsymbol{NP}$ problems. It is notable to mention the Traveling Salesman Problem (TSP) Flood (1956); Croes (1958), one of the most famous problems in this category, due to its continuous relevance and wide applicability in various optimization and logistics scenarios.

The Traveling Salesman Problem (TSP) exemplifies NP-hard problems in combinatorial optimization. Formally, given a set of n cities $\{C_1, C_2, \ldots, C_n\}$ and a distance matrix $D = [d_{ij}]$, where d_{ij} represents the distance between cities C_i and C_j, the objective is to find a permutation π of the cities that minimizes the total travel distance:

$$\text{Minimize } \sum_{i=1}^{n-1} d_{\pi(i)\pi(i+1)} + d_{\pi(n)\pi(1)}. \tag{1}$$

The complexity of TSP is factorial, $\mathcal{O}(n!)$, making exact solutions computationally infeasible for large n due to the combinatorial explosion (Applegate et al., 2007). The practical applications of TSP are vast, including logistics, where it optimizes delivery routes, and manufacturing, where it sequences tasks efficiently.

Solving the largest Traveling Salesman Problem (TSP) instance to date, involving 85,900 cities, took several months. This achievement by David Applegate, Robert Bixby, Vašek Chvátal, and William Cook utilized advanced mathematical techniques and high-performance computing Applegate et al. (2009).

Hence, with the advent of quantum computing, quantum annealing offers a new paradigm for optimization. Quantum annealing, a metaheuristic technique inspired by simulated annealing and leveraging quantum mechanical phenomena, is a promising approach for solving NP-hard problems. It operates by encoding an optimization problem into an Ising model or a Quadratic Unconstrained Binary Optimization (QUBO) problem. The goal is to find the ground state of the Hamiltonian representing the problem. For an Ising model, the problem is formulated as:

$$H = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z, \tag{2}$$

where σ_i^z are the Pauli Z operators representing spin states, h_i are external magnetic fields, and J_{ij} are the interaction strengths between spins. In the QUBO formulation, the objective is to minimize:

$$\text{Minimize } \mathbf{x}^T Q \mathbf{x}, \tag{3}$$

where $\mathbf{x} \in \{0, 1\}^n$ is a binary vector and Q is an upper triangular matrix encoding the problem. Quantum annealers, such as those developed by D-Wave Systems Inc., aim to evolve the system from an initial superposition state to the ground state, which ideally corresponds to the optimal solution of the encoded problem (Kadowaki & Nishimori, 1998; McGeoch & Wang, 2013).

Despite advancements, efficient solutions for TSP using quantum annealing remain elusive. Prior research, such as the study by (Jain, 2021), illustrated the potential of using D-Wave's quantum annealers for TSP by reformulating it as a QUBO problem. However, their results indicated that the quantum solver was limited to small instances (up to 8 nodes) and exhibited suboptimal performance compared to classical heuristic solvers. This highlights the current limitations of quantum annealing in addressing larger and more complex instances of TSP.

In this paper, we propose an innovative approach to solving the TSP using the latest advancements in D-Wave's quantum annealing technology. By using the enhanced capabilities of the newest Advantage quantum processor, featuring over 5000 qubits with the fast annealing feature (McGeoch & Farre, 2023), our study reformulates TSP as a QUBO problem and utilizes this advanced quantum hardware.

Our main contribution lies in conducting a comprehensive analysis of the current state of quantum annealing for solving TSP and proposing enhancements to overcome limitations identified in prior studies. By systematically comparing quantum solutions with classical heuristic solvers, we aim to assess the efficacy of these advancements and identify the strengths and weaknesses of contemporary quantum annealing techniques. Furthermore, we show the time complexity aspects of classical versus quantum approaches.

This research significantly contributes to the understanding of quantum computing applications in combinatorial optimization, offering insights into the practical capabilities and constraints of modern quantum hardware. It provides valuable guidance for future developments in quantum optimization methodologies and supports the ongoing quest for efficient solutions to complex NP-hard problems.

2 Background

Quantum annealing is an advanced computational technique employed to solve optimization problems by harnessing the principles of quantum mechanics. Unlike classical annealing, which relies on thermal fluctuations to explore the energy landscape of a problem, quantum annealing uses quantum tunneling to escape local minima and potentially locate the global minimum more efficiently Morita & Nishimori (2008); Rajak et al. (2023); Yarkoni et al. (2022).

In quantum annealing, an optimization problem is encoded into a Hamiltonian, which represents the system's energy landscape. The system is then evolved from a simple initial Hamiltonian to a problem-specific Hamiltonian. This process is governed by the Schrödinger equation, and the system is cooled quantum mechanically to find the ground state, which corresponds to the optimal solution of the problem.

The Hamiltonian $H(t)$ during the quantum annealing process is a time-dependent operator defined as:

$$H(t) = A(t)H_0 + B(t)H_p \tag{4}$$

where:

- H_0 is the initial Hamiltonian, often chosen to be a simple Hamiltonian that can be easily prepared.
- H_p is the problem Hamiltonian, encoding the optimization problem.
- $A(t)$ and $B(t)$ are time-dependent functions that control the evolution of the Hamiltonian, with $A(t)$ typically decreasing and $B(t)$ increasing over time.

The objective is to find the ground state of H_p by starting with the ground state of H_0. The system undergoes quantum evolution governed by the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \tag{5}$$

where $|\psi(t)\rangle$ is the quantum state of the system at time t, and $\hbar$ is the reduced Planck constant.

The process of quantum annealing can be broken down into several key stages Salloum et al. (2024):

1. **Initialization:** The system is initialized in the ground state of the initial Hamiltonian H_0, which is typically chosen to be a simple Hamiltonian, such as one corresponding to a transverse field.
2. **Annealing Schedule:** The functions $A(t)$ and $B(t)$ are designed to slowly interpolate from H_0 to H_p over time. This gradual evolution ensures that the system remains in its ground state, according to the adiabatic theorem.
3. **Quantum Evolution:** During the annealing process, quantum tunneling allows the system to explore the energy landscape more thoroughly than classical thermal fluctuations. This can enable the system to bypass local minima and move towards the global minimum.

4. **Measurement:** At the end of the annealing schedule, the final Hamiltonian H_p represents the problem to be solved. The system is measured, and the resulting state corresponds to the optimal or near-optimal solution of the original optimization problem.

Quantum annealing is particularly effective for problems that can be mapped into a Quadratic Unconstrained Binary Optimization (QUBO) formulation or an Ising model. These formulations are versatile and can represent a wide range of combinatorial optimization problems, making quantum annealing a powerful tool in the field of optimization.

3 PROBLEM FORMLUATION: TSP AS A QUBO

TSP as we mentioned before is a classic combinatorial optimization problem. The objective is to find the shortest possible route that visits a set of cities exactly once and returns to the origin city. Below, we develop the QUBO formulation for the TSP. Let q_{ij} be a binary variable, where $q_{ij} = 1$ if city i is visited at step j, and $q_{ij} = 0$ otherwise.

The objective is to minimize the total travel distance. Let d_{ik} represent the distance between city i and city k. The objective function can be expressed as:

$$\text{Minimize} \quad \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} d_{ik}\, q_{ij}\, q_{k((j+1) \bmod n)} \tag{6}$$

Here, $j + 1 \mod n$ ensures that the tour returns to the origin city after the last step. To ensure a valid tour, we impose the following constraints:

EACH CITY MUST BE VISITED EXACTLY ONCE

$$\sum_{j=0}^{n-1} q_{ij} = 1 \quad \forall\, i \in \{0, 1, \ldots, n-1\} \tag{7}$$

EACH TIME STEP MUST HAVE EXACTLY ONE CITY VISITED

$$\sum_{i=0}^{n-1} q_{ij} = 1 \quad \forall\, j \in \{0, 1, \ldots, n-1\} \tag{8}$$

To translate these constraints into a QUBO formulation, we introduce penalty terms for each constraint and combine them with the objective function. For each city i, the sum of q_{ij} over all j must be exactly 1. The penalty term for this constraint is:

$$\lambda_1 \sum_{i=0}^{n-1} \left(\sum_{j=0}^{n-1} q_{ij} - 1 \right)^2 \tag{9}$$

For each time step j, the sum of q_{ij} over all i must be exactly 1. The penalty term for this constraint is:

$$\lambda_2 \sum_{j=0}^{n-1} \left(\sum_{i=0}^{n-1} q_{ij} - 1 \right)^2 \tag{10}$$

Combining the objective function and penalty terms, we obtain the total QUBO formulation:

$$Q(x) = \sum_{j=0}^{n-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} d_{ik} q_{ij} q_{k((j+1) \bmod n)} + \lambda_1 \sum_{i=0}^{n-1}\left(\sum_{j=0}^{n-1} q_{ij} - 1\right)^2 + \lambda_2 \sum_{j=0}^{n-1}\left(\sum_{i=0}^{n-1} q_{ij} - 1\right)^2 \quad (11)$$

where λ_1 and λ_2 are Lagrange multipliers that penalize constraint violations.

By fixing the start of the tour at city 0 (i.e., q_{00} is always 1), we can simplify the formulation. This reduction assumes that the tour forms a cycle, so the starting point does not affect the optimal solution.

The refined QUBO formulation is:

$$Q'(x) = \sum_{j=1}^{n-2}\sum_{i=1}^{n-1}\sum_{k=1}^{n-1} d_{ik} q_{ij} q_{k(j+1)} + \sum_{i=1}^{n-1}(d_{0i}q_{i1} + d_{i0}q_{i(n-1)}) + \lambda_1 \sum_{i=1}^{n-1}\left(\sum_{j=1}^{n-1} q_{ij} - 1\right)^2 + \lambda_2 \sum_{j=1}^{n-1}\left(\sum_{i=1}^{n-1} q_{ij} - 1\right)^2$$

The indices i and j start from 1 because city 0 is fixed at the start. Additionally, the second term in the refined QUBO formulation accounts for the distances from the first city (0) to the second city and from the last city back to the first city. This trick will reduce the size of our QUBO matrix from $n \times n$ to $(n-1) \times (n-1)$.

4 Experiments and Results

We conducted a series of experiments utilizing the D-Wave quantum annealer Boothby et al. (2020) (QPU) and the Hybrid Solver (HQPU), specifically utilizing the "Pegasus" architecture provided by the Advantage 4.1 device. Complementary to this, classical computations were executed on an Intel(R) Core(TM) i5-8250U CPU @ 1.60GHz.

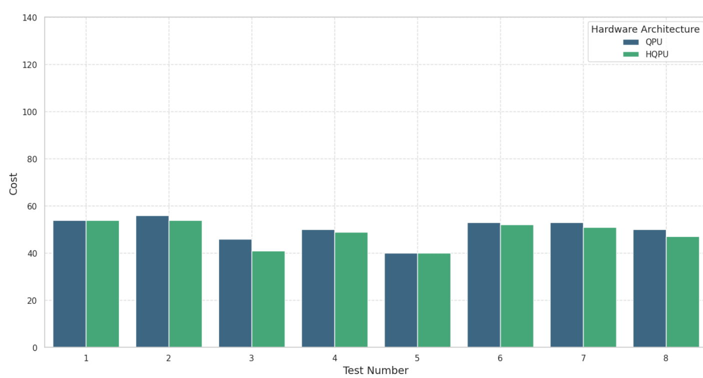

Figure 1: EQATS Results for Hardware Architecture for the 8 cities problem case

The HQPU combines classical heuristics with D-Wave's quantum annealer to efficiently solve complex problems within time constraints. It features a front end that receives problem inputs and time limits, then launches multiple heuristic solvers on classical CPUs and GPUs. Each solver includes a quantum module

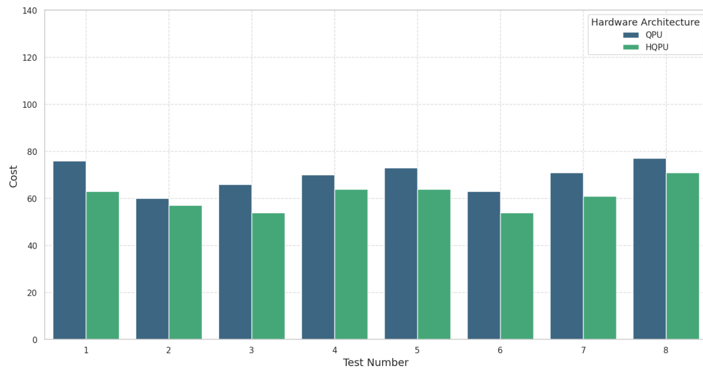

Figure 2: EQATS Results for Hardware Architecture for the 9 cities problem case

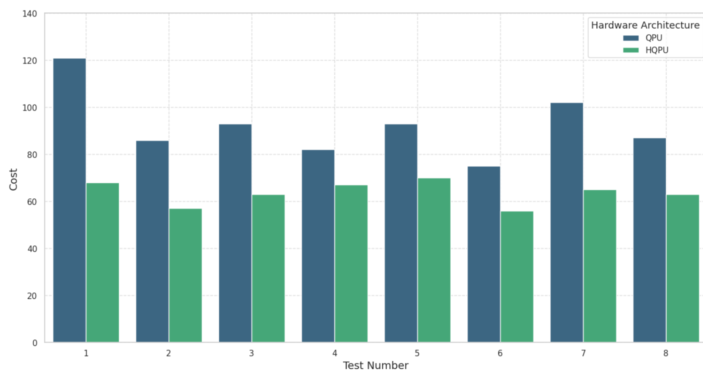

Figure 3: EQATS Results for Hardware Architecture for the 10 cities problem case

(QM) that interfaces with the D-Wave QPU. Quantum queries from QMs are processed by the QPU using quantum annealing to explore complex solution landscapes. The system integrates insights from both classical and quantum methods, enhancing the search process. Results are aggregated and refined by a portfolio management component to present a high-quality subset of solutions to the user.

Initially, we compared our proposed formulation on the QPU and HQPU. As shown in Figures 1, 2, and 3, the HQPU demonstrated significantly higher efficiency. Consequently, we will proceed with comparing our formulation using the HQPU. The primary objective of these experiments was to solve instances of the TSP for datasets comprising 8, 9, and 10 cities, comparing our approach with the D-Wave approach and the approaches in Jain (2021). The outcomes of these experiments aim to offer a comparative analysis, as shown in Figures 4, 5, and 6, shows the performance between quantum and classical computational approaches for this complex optimization problem.

We additionally implemented a backtracking algorithm to ensure that we have a baseline, as backtracking guarantees an optimal solution. For each instance, we conducted 8 different experiments. Our approach ”EQATS” consistently achieved the optimal solution, unlike Jain’s proposed quantum solver. Notably, the cost was very high, especially for the 10-cities problem case, where only once did it provide a solution, and that solution had a very high cost. To compare our work with the D-Wave TSP solver D-Wave Systems

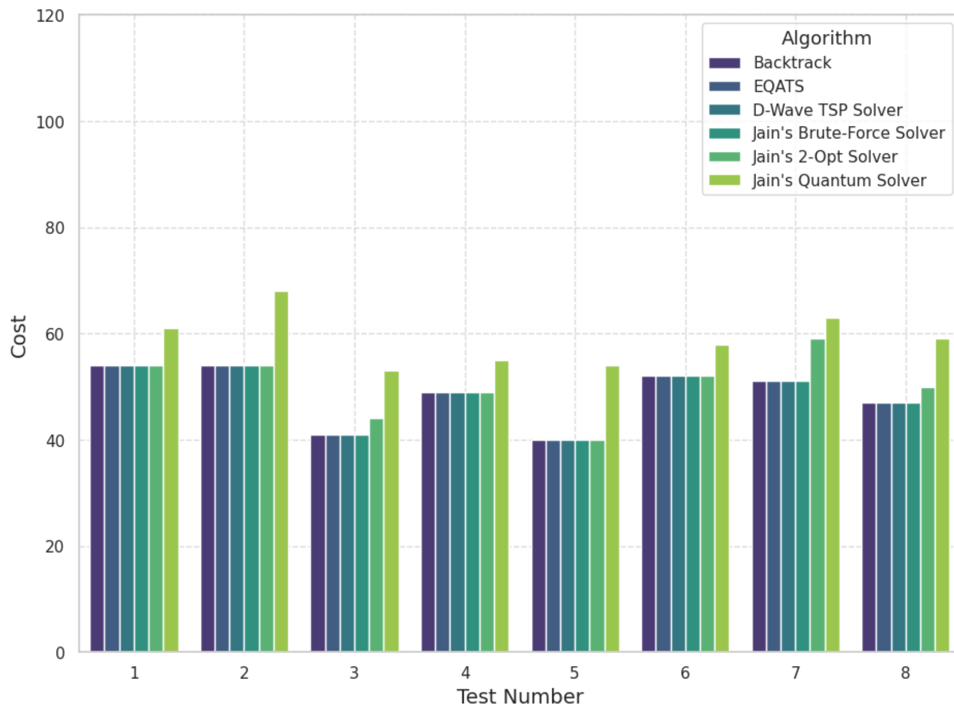

Figure 4: Results of the Algorithms for the 8 cities problem case

(2024), we conducted 8 different experiments for the 20-cities case. As shown in Figure 7, we outperformed the D-Wave TSP solver by approximately 35%.

5 Discussion

Our approach, EQATS, consistently achieved optimal solutions across datasets of 8, 9, and 10 cities. This demonstrates its robustness and effectiveness. Notably, EQATS outperformed the D-Wave TSP solver by approximately 35% in the 20-cities case, highlighting the significant advantage of our method in handling larger problem instances. The hybrid quantum-classical approach, represented by the HQPU, also showed superior performance compared to the QPU. This advantage underscores the efficacy of combining quantum and classical computations, enhancing both efficiency and scalability for complex optimization problems like the TSP. Jain's proposed quantum solver faced issues with high costs and inconsistent performance, especially with larger datasets, indicating that existing quantum methods may not yet be fully optimized for large-scale TSP problems. While our EQATS approach and the hybrid quantum-classical methods demonstrate clear advantages, including achieving optimal solutions and outperforming current quantum solvers, challenges remain. Future work should focus on scaling our approach to even larger datasets, optimizing the hybrid algorithm, and exploring the specific components of the HQPU that contribute to its performance. Additionally, advancing quantum solvers and improving hardware integration will be crucial for overcoming current limitations and furthering the field of quantum computing in optimization problems.

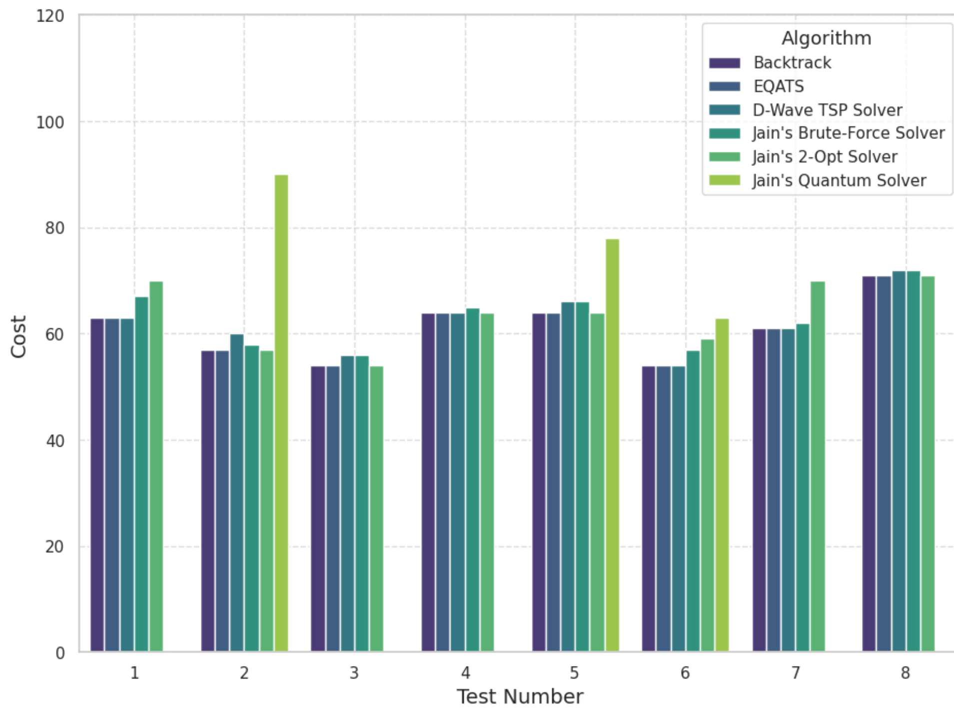

Figure 5: Results of the Algorithms for the 9 cities problem case

6 CONCLUSION & FUTURE WORK

This study evaluated various computational methods for solving the Traveling Salesman Problem (TSP), including our EQATS approach, the D-Wave quantum annealer (QPU), the Hybrid Solver (HQPU) using the Pegasus architecture, and classical methods. Our EQATS approach consistently provided optimal solutions and outperformed the D-Wave TSP solver by approximately 35% for the 20-cities case, demonstrating its effectiveness in handling larger datasets. The HQPU also showed superior performance compared to the QPU, highlighting the benefits of hybrid quantum-classical approaches in enhancing efficiency and scalability. However, limitations such as high costs and inconsistent performance with current quantum solvers, including Jain's methods, were noted. Our results underscore the advantages of hybrid quantum-classical methods and our EQATS formulation in optimizing TSP solutions. Future work will involve conducting robust experiments across various cases and on a larger scale to further demonstrate the capabilities of quantum annealing. These experiments will compare the performance of quantum annealers with more classical algorithms, providing a comprehensive assessment of their effectiveness in solving complex optimization problems. The focus will be on scaling these methods, refining hybrid algorithms, and addressing hardware limitations to further advance quantum computing in the realm of complex optimization problems.

DATA AND CODE AVAILABILITY

For transparency and reproducibility, the code and datasets used in this study are publicly available. You can access them at `https://github.com/anasalatasiuni/QuantumTravelingSalesmanSolver`.

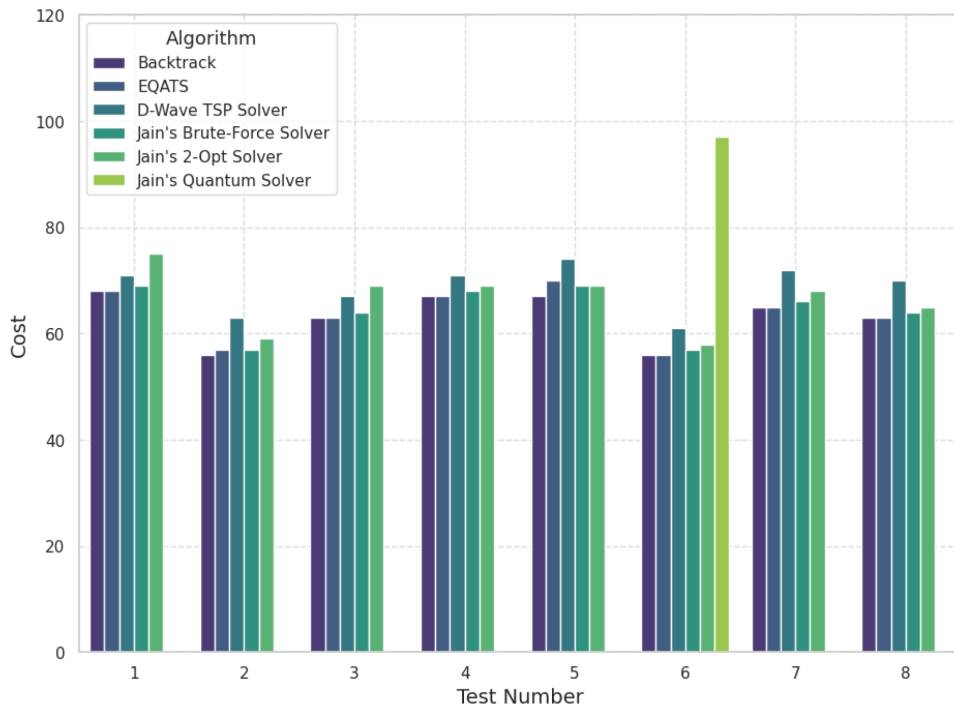

Figure 6: Results of the Algorithms for the 10 cities problem case

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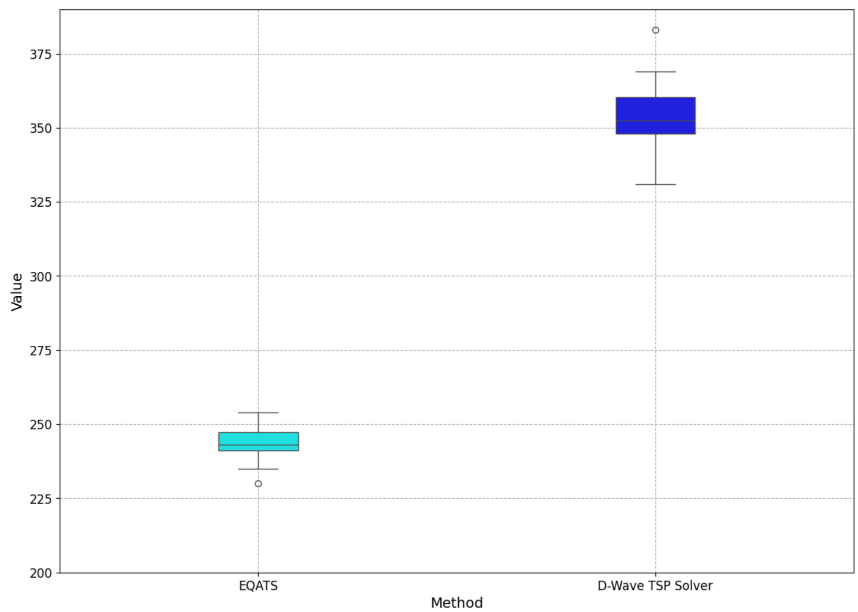

Figure 7: EQATS vs D-Wave TSP Solver for the 20 cities problem case

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A DETAILED ANALYSIS OF THE EIGHT-CITY TSP CASE

The Traveling Salesman Problem (TSP) was analyzed for a graph consisting of 8 cities, with the distance matrix provided in Figure 8:

$$\begin{matrix} 0 & 5 & 3 & 1 & 5 & 1 & 7 & 8 \\ 7 & 0 & 6 & 4 & 4 & 4 & 6 & 7 \\ 4 & 7 & 0 & 5 & 5 & 7 & 8 & 2 \\ 4 & 2 & 3 & 0 & 4 & 5 & 3 & 6 \\ 1 & 4 & 8 & 3 & 0 & 5 & 8 & 1 \\ 3 & 3 & 4 & 7 & 1 & 0 & 6 & 1 \\ 4 & 7 & 2 & 7 & 1 & 8 & 0 & 5 \\ 4 & 8 & 6 & 5 & 5 & 3 & 3 & 0 \end{matrix}$$

Figure 9 illustrates the Q matrix embedding for the D-Wave quantum annealer, while Figure 10 displays the energy distribution of the solutions.

Figure 11 presents the optimal solution for the eight-city TSP case.

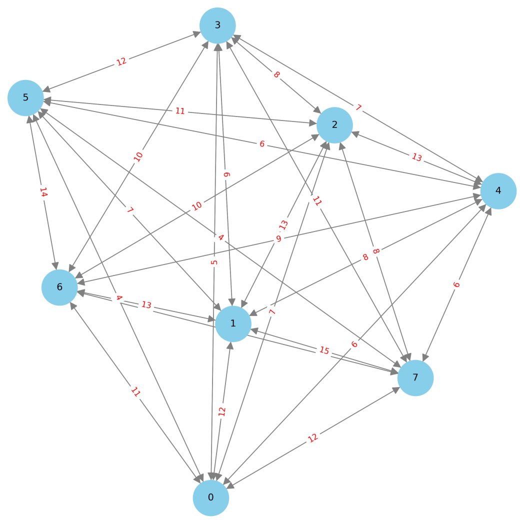

Figure 8: Distance matrix for the eight-city TSP graph.

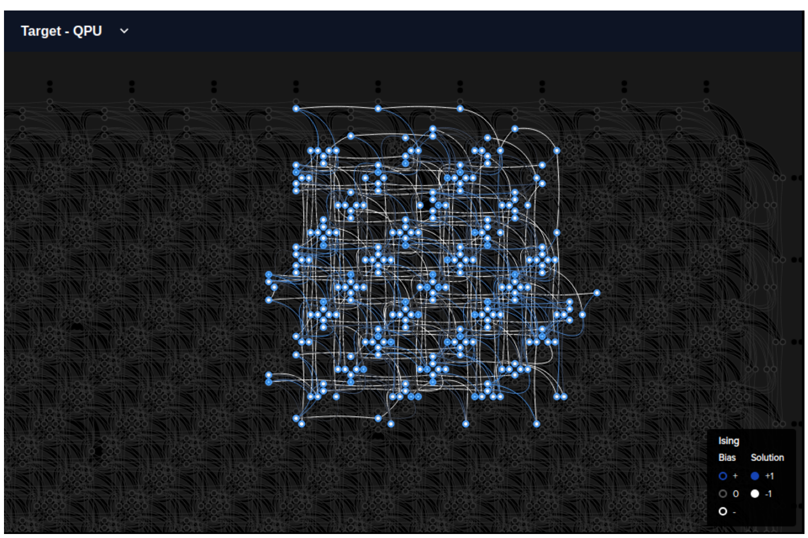

Figure 9: Q matrix embedding on the D-Wave quantum annealer for the eight-city TSP.

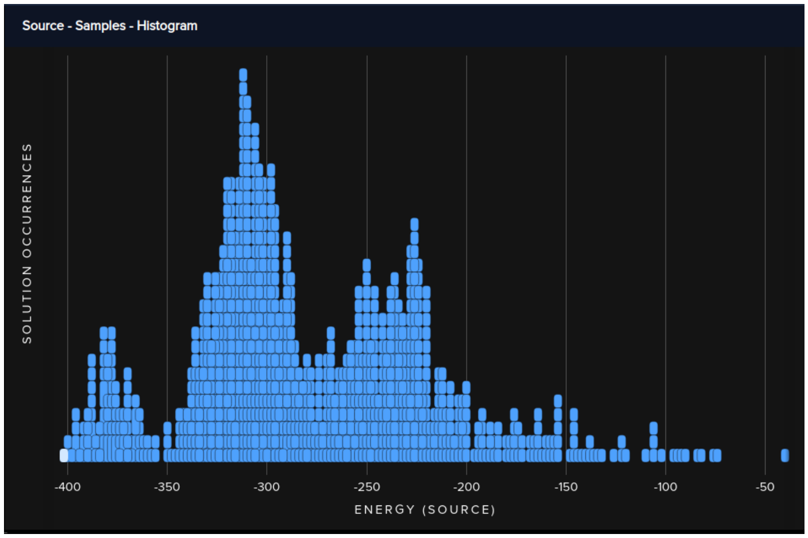

Figure 10: Energy distribution of solutions for the eight-city TSP.

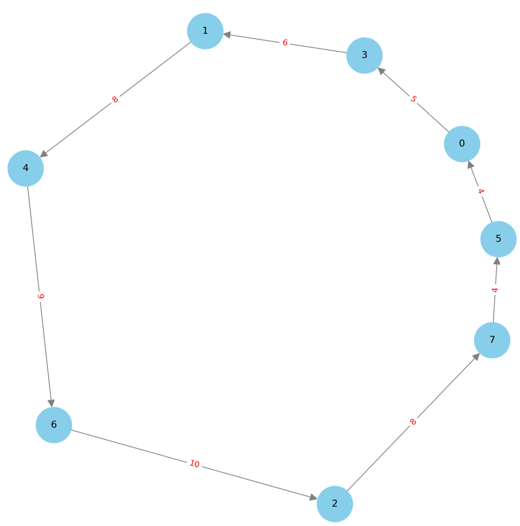

Figure 11: Optimal solution for the eight-city TSP.