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Evaluating quantum-classical heuristics for traveling salesman problem

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Abstract. In this paper, we develop and evaluate a hybrid quantum-classical heuristic approach to solving the Traveling Salesman Problem. This approach uses exhaustive enumeration of the starting paths and optimizes the remainder of the route using quantum computing. For quantum co-processing, we use either the Variational Quantum Eigensolver or the Quantum Annealing. Results of evaluation of the approach on several datasets including TSPLIB and touristic data for Petrozavodsk and Karelia Republic, both in simulation and in hardware, are presented. Issues of practical applicability are also discussed.

Key words and phrases: hybrid quantum-classical heuristics, traveling salesman problem, variational quantum eigensolver, quantum annealing

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1. Introduction

Traveling Salesman Problem (TSP) is a challenging combinatorial problem which is NP-hard [1], that is, the exact optimal solution in general cannot be obtained in polynomial time (w.r.t. the size of input data). The problem implies a search for the shortest possible (cyclic) route that visits (exactly once) a set of cities and returns to the starting city. Since the number of feasible routes increases exponentially with the number of cities [2], it is computationally hard to solve for large TSP instances using traditional algorithms such as brute force and the Held–Karp algorithm [3] (which, however, works well on a small scale).

Despite its difficulty, the TSP has many practical applications in various fields such as logistics [4], transportation, and network design. Finding efficient solutions to TSP can help industries optimize delivery routes, reduce costs, and improve overall efficiency. Due to this practical importance, various heuristic and approximation algorithms were introduced to find suboptimal solutions in a reasonable time, such as the nearest-neighbor search [5] or k-opt [6] for the Lin–Kernighan algorithm [7]. The search for effective algorithms continues, and new promising efforts are made in the direction of novel computing hardware such as quantum computing (QC).

This research is focused on solving the TSP with QC techniques. QC is a promising research field for solving large-scale problems due to the so-called *quantum supremacy*. The latter is a theoretical concept that exploits quantum bit (qubit) properties such as quantum *superposition* (co-existence of the qubit in multiple states at once) and *entanglement* (dependence of several qubits) to outperform traditional algorithms. Some examples of effective quantum algorithms include the celebrated Shor algorithm [8] and Deutsch–Josa algorithm [9], the latter being a key example of the so-called *quantum parallelism* [10]. Performance of such effective schemes is, however, limited due to the need of a quantum-classical input-output interface and imperfections of the present QC hardware such as limited coherence time due to environmental noise, high error rates and a relatively small number of qubits, those being problems of the so-called Noisy intermediate-scale quantum (NISQ) computers [11].

One of the natural classes of problems that can be addressed by QC is optimization, and in many cases the QC techniques can either offer speedup to the classical algorithms, or deliver efficient heuristics. A detailed description of state-of-the-art quantum optimization (QO) methods, both from the perspective of complexity and practical applicability, is given in the review paper [2]. Two important QO techniques are the Variational Quantum Algorithms (VQA) [12, 13] and Quantum Annealing (QA) implemented on hardware [14]. While the former allows one to use gate and circuit-based QC hardware (known to be *universal* i.e. capable of running any algorithm), the latter suits only for QA machines such as the D-Wave, useful only for a specific problem set. However, both options can be effectively used to tackle the class of Quadratic Unconstrained Binary Optimization (QUBO) problems where the cost function is quadratic w.r.t. the binary unknowns.

Within QO, TSP is a prominent example of a problem in which complexity depends on specific requirements and restrictions (such as the type of state space and the goal), and heuristic QO can provide meaningful results even if quantum speedups seem unattainable [2]. Thus, many researchers focus on solving TSP using various heuristic QO algorithms, including QA and VQA. We briefly summarize these two key approaches to TSP below, and refer the interested reader to a survey [15] that outlines general logistics and supply chain management problems treated by QC.

In [16], a comparative study of Quantum Approximate Optimization Algorithms (QAOA), a specific variant of VQA, is performed. Various aspects of the approach, such as sensitivity to the TSP graph, numerical accuracy and effect of noise, are studied. Performance of QAOA implementation for TSP with 5 cities is studied in [17]. In [18], comparative study of solution encoding is performed for the TSP problem to be solved using VQA methods. Results are presented for problem sizes of up to 6 cities. In [19], Variational Quantum Eigensolver (VQE), which is another representative of VQA class, and QAOA schemes are compared to the approach based on the so-called Grover adaptive search, and numerical results are presented for TSP with up to 7 cities. The effect of the various configurations of the parametrized quantum circuits within the VQE approach to TSP is demonstrated in [20], and numerical results are presented for 4-cities TSP.

In [21], QA was used to tackle TSP with four smallest problems from TSPLIB including Burma14 by the D-Wave using Kerberos and LeapHybridSampler solvers, and reasonable solution quality was reported with relatively less optimal solutions found for bigger size problems. Note, however, that the solvers used are hybrid (quantum-classical) and remain trade secrets of the D-Wave [21]. In contrast,

D-Wave's 5,000-qubit Advantage 1.1 quantum annealer is useful only for solving TSP with 8 or fewer cities, as reported in [22]. A groundbreaking approach in solving TSP by minimal QC resources was introduced in [23], where a single-qubit scheme with a careful encoding of TSP using Bloch sphere was used to obtain solutions with problem size up to 9. We also mention that solving TSP by QA can be a useful part of a hybrid approach to more general real-time routing problem [24].

In summary, both in the VQA and QA approaches to TSP the size of the problem that is solvable by QC is rather limited, which is in part explained by the imperfections of the NISQ hardware [25]. In most cases reported in the literature reviewed above, the size of the TSP solved by the QC hardware is at most 9 cities. At the same time, hybrid approaches such as the one in [21] are useful for studying larger problems. This motivates us to develop a hybrid quantum-classical approach to TSP that can be used both within the QA and VQA frameworks. To do so, we use the QUBO representation of the TSP. The key ingredients of our approach are the classical enumeration of the beginning of the route followed by QC counterpart used as the co-processor to optimize the route ending. This novel combination is the key contribution of the present paper.

Following [25], we use VQE as the VQA class technique, and we use D-Wave in case of the QA. We demonstrate the capabilities of our approach using TSPLIB example and apply the method to optimize tours between points of interest (POI) within Karelia Republic and Petrozavodsk city.

The rest of the paper is organized as follows. We give a necessary background on the QC, VQE and QA, describe the QUBO representation of the TSP in Section 2. The hybrid approach for solving TSP in QUBO form is proposed and evaluated (using the TSPLIB dataset Burma14 and a few others) in Section 3. The paper ends up with a discussion on possible complications with solving TSP in QUBO form in Section 4.

2. Necessary Background

In this section we briefly review the QC and QO fundamentals, TSP and its QUBO representation. This information is useful for the development of the hybrid approach. More detailed information on QC can be found in the celebrated monograph [26], and QO is reviewed in [2]. We also refer the reader to the book [27] for a more concise view of TSP.

2.1. QC Fundamentals

A qubit is a basic information unit in QC. It is a quantum system with two basis states $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ living in a 2-dimensional Hilbert space. Any qubit state $|\psi\rangle$ can be in *superposition* of the basis states, meaning that

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \quad \alpha, \beta \in \mathbb{C}, \;\; |\alpha|^2 + |\beta|^2 = 1.$$

The coefficients α and β hold a defined physical significance, as observing a qubit would result in the state $|0\rangle$ with probability $|\alpha|^2$ and $|1\rangle$ with probability $|\beta|^2$. However, a qubit can only be measured once as the measurement process causes the qubit to collapse to one of the binary states, preserving that state in subsequent measurements. (Using Dirac notation, $|\psi\rangle$ is a column, and $\langle\psi|$ is a row vector of appropriate size.)

To compose multiple independent qubits, the tensor (Kronecker) product $\otimes$ is typically used. For example, the product $\psi \otimes \varphi$ of two single-qubit states $|\psi\rangle$ and $|\varphi\rangle$ results in a qubit pair state represented as a vector in $\mathbb{C}^4$, and in general n qubits can be represented as a vector in $\mathbb{C}^{2^n}$. Such a representation can be written as

$$|\varphi\rangle = \sum_{i=0}^{2^n} \alpha_i |i\rangle,$$

where $\sum_{i\leq 2^n} |\alpha_i|^2 = 1$ and $\alpha_i \in \mathbb{C}$. The basis vectors $|i\rangle$ can also be written in the form of binary representation of i from the set $\{0,1\}^n$, say, $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$ instead of $|0\rangle, \dots, |3\rangle$ for $n = 2$. However, algebraically, the size of $|\phi\rangle$ and, correspondingly, $|i\rangle$ is 2^n, where we can write

$$|i\rangle = (x_0, \dots, x_{2^n}), \quad x_j = \delta_{i,j}, \tag{1}$$

with $\delta_{i,j} = 1$ for $i = j$ and 0 otherwise (i.e. Kronecker delta function).

Note that states of qubits that can be represented as the tensor product are independent. On the contrast, *entanglement* allows qubits to interact regardless of their distance, creating a strong connection between them. When qubits are entangled, they cannot be treated separately and their states become dependent on each other. The Bell state of a 2-qubit system

$$|\varphi\rangle = \frac{|00\rangle + |11\rangle}{2}$$

is an example where the state cannot be broken down into two separate single-qubit states.

2.2. QC Models

There are two widely used models of QC. The universal model (that can represent any computation) is constructed by using the *quantum gates* which act on individual qubits and their groups. In QC hardware, these gates usually operate with single qubits and pairs. Such operations can be interpreted as matrix multiplications from the left by the unitary matrix U. A matrix U is unitary if its conjugate (Hermitian) transpose equals its inverse, $U^* = U^{-1}$. Note that such a transformation preserves matrix norms, and thus keeps the unit sum of probabilities for the qubit states after transpose. Using quantum gates and qubits, the quantum program is often represented as the so-called quantum circuit which describes the sequence of gates applied to various *qubit lines* (acting as variables, e.g. inputs or outputs of the program). In such a model, input is transformed into output by a sequence of gates in a discrete way.

Another universal model is the so-called adiabatic QC (AQC). On the contrast to the circuit model, in AQC the transformation of the qubit state to the desired solution of the problem is performed continuously, by slow change in the parameters of the system Hamiltonian $H(t)$ at time t (in AQC hardware it can be implemented, say, by a slowly changing magnetic field). Due to a slow change, the qubits remain in the so-called *ground state* (i.e. state with minimal energy) which corresponds to the system Hamiltonian $H(t)$. Thus, to obtain the desired solution, problem is encoded in a Hamiltonian H_P whose minimal energy state is the desired solution, and the transformation is organized by a scheme

$$H(t) = (1 - s(t))H_I + s(t)H_P, \;\; t \in [0, \tau], \tag{2}$$

where $s : [0, \tau] \to [0, 1]$ is a smooth monotone function such that $s(0) = 0$ and $s(\tau) = 1$, H_I is some initial Hamiltonian which is easy to construct, and τ is the final time of computation. It can be noted that the solution of a problem in AQC is obtained in finite time τ irregardless of the properties of H_P.

2.3. VQA and VQE

VQA is a class of algorithms that adopt hybrid quantum-classical approach to obtain quantum advantage on the NISQ devices [12]. This set is universal in a sense that arbitrary quantum circuit can be represented by an appropriate VQA problem [28]. The approach is based on defining a cost function $C(\theta)$ which encodes the problem and estimating $C(\theta)$ by QC, whereas classically optimizing θ, to find $\theta^* = \text{argmin}_\theta\, C(\theta)$ (encoding the solution). Dependence on θ is parametrized by the so-called ansatz operator $U(\theta)$, a specific quantum operator which is then optimized iteratively.

A specific version of VQA is VQE aimed at finding the ground state energy of quantum systems [29]. This makes it particularly valuable in quantum chemistry [30], materials science [31], and chemical engineering [32]. The algorithm is based on AQC approach [33] and the variational principle. According to the latter, for any system represented by the Hamiltonian H and the quantum state $|\psi\rangle$, the expectation value $\langle\psi|H|\psi\rangle$ (corresponding to the expected energy value of the system) is equal to or greater than the ground state energy of the system [34]. It is interesting to illustrate, why $\langle\psi|H|\psi\rangle$ is the expected value of the energy that is obtained after measurement. Indeed, take $|\psi\rangle = \sum_{i=0}^{2^n} \alpha_i |i\rangle$ and use the so-called Hermitian decomposition [35] to obtain $H = \sum_{i=0}^{2^n} \lambda_i |i\rangle\langle i|$, where λ_i are eigenvalues corresponding to eigenvectors $|i\rangle$ and $\langle i|$ (these correspond to energy states of the appropriate basis states). Note that due to (1), the basis $|0\rangle, \dots, |2^n\rangle$ is orthonormal. Then, recalling that $\langle x|y\rangle$ is the complex scalar product that requires complex conjugate to be used on the first argument, observe

$$\langle\psi|\, H\, |\psi\rangle = \sum_{i=0}^{2^n} \lambda_i \langle\psi|i\rangle\langle i|\psi\rangle = \sum_{i=0}^{2^n} \lambda_i \alpha_i^* \alpha_i. \tag{3}$$

Recalling that $\alpha_i^*\alpha_i = |\alpha_i|^2$ is the probability of measuring the basis state $|i\rangle$, it is clear from (3) that the value observed corresponds to the average energy of the system.

Since in VQE the value ψ depends on the parameter vector θ, after measuring the average energy $C(\theta) = \langle\psi(\theta)|\, H\, |\psi(\theta)\rangle$, the value θ is iteratively modified so as to minimize $C(\theta)$ and, accordingly, minimize the energy of the ground state of the system [12, 29]. To achieve this, VQE uses QC to initialize quantum register ψ_0, apply anzatz to get $\psi(\theta) = U(\theta)\psi_0$, then apply H and measure $C(\theta)$, and optimize the circuit's parameter θ variationally (using classical optimizer) by repeating these steps accordingly.

2.4. QA

A particular case of AQC, which is not universal, but rather useful in QO, is QA. Historically the QA term was also used to denote heuristic optimization method [36] (which is somewhat similar to the so-called simulated annealing). To be analyzed by QA, the (optimization) problem needs to be encoded by a Hamiltonian H_P in such a way that the ground state (with minimal energy) of a system characterized by H_P corresponds to the desired solution. Then the solution is obtained using the sufficiently slow evolution of the ground state from the one encoded by initial Hamiltonian H_I following (2). The initial Hamiltonian H_I is selected in such a way that the ground state is relatively straightforward, say, when all qubits are in a superposition state $|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. Hardware implementations such as the D-Wave machine in the majority of cases require H_P to represent quadratic model, that is, to have the Ising form or QUBO form. In the former case,

$$H_P = \sum_{i=1}^{n} h_i {\sigma_z}^i + \sum_{i>j} J_{ij} {\sigma_z}^i {\sigma_z}^j, \tag{4}$$

where ${\sigma_z}^i = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ is the so-called Pauli-Z matrix acting on qubit $i = 1, \dots, n$, $J_{ij} = J_{ji}$ is the so-called coupling strength of the coupled qubits i and j and h_i is the so-called qubit bias (on-site energy) acting on qubit i. The matrix ${\sigma_z}^i$ has eigenvalues $\{-1, 1\}$ and thus, using QA, the Ising cost function is minimized [37]:

$$\mathcal{E}() = \sum_{i=1}^{n} h_i z_i + \sum_{i>j} J_{ij} z_i z_j, \tag{5}$$

where $\in \{-1, 1\}^n$. In D-Wave systems, $h_i \in [-2, 2]$ and $J_{ij} \in [-1, 1]$ (these ranges, however, can be extended by autoscaling). When running the optimization problem on a QA machine, the topology of possible coupling between qubits needs to be taken care of, which can be done automatically by the so-called minor embedding. This process, however, may dramatically upscale the problem in terms of the number of physical qubits required.

In summary, the optimization problem is encoded by the vector $(h_1, \dots, h_n)$ and the matrix $||J_{i,j}||_{i,j\in\{1,\dots,n\}}$, and the solution needs to be decoded from the vector $\vec{z} \in \{-1, 1\}^n$ that minimizes the Ising cost $\mathcal{E}(\vec{z})$ given in (5).

An equivalent representation of the problem is in QUBO format, where the solution is encoded by a binary vector. In such a case, QUBO objective function has the following form:

$$\mathcal{E}(\vec{x}) = \vec{x}^T Q \vec{x} = \sum_{i=1}^{n} Q_{ii} x_i + \sum_{i>j} Q_{ij} x_i x_j, \tag{6}$$

where $\vec{x} \in \{0, 1\}^n$. Therefore, the optimal solution in QUBO format is $\operatorname{argmin}_{\vec{x}} \mathcal{E}(\vec{x})$, where $\vec{x}$ is a binary vector encoding the solution, and Q is a symmetric matrix of real values encoding the problem.

2.5. TSP and its QUBO Representation

There are many ways to define the problem in TSP class, depending on the restrictions imposed, goals to optimize and properties of the travel costs. In simpler case, the cost of travel from city $i = 1, \dots, n$ to $j = 1, \dots, n$ is symmetric, i.e. equals the cost from j to i, and these constitute a matrix $M = ||M_{ij}||_{i,j\le n}$, where $M_{ij} = M_{ji}$. Then it is straightforward to define the cost of a tour with the help of a binary matrix $X = ||X_{ij}||_{i,j\le n}$, where $X_{ij} = 1$ if i-th city is traversed at j-th place. As such, the cost of travel can be given as

$$\sum_{k=1}^{n-1} \sum_{i=1}^{n} \sum_{j=1}^{n} M_{ij} X_{ik} X_{j(k+1)} + \sum_{i=1}^{n} \sum_{j=1}^{n} M_{ij} X_{in} X_{j1}. \tag{7}$$

Unrolling the matrix X columnwise into a column vector $\vec{x} = (x_1, \dots, x_{2^n})$ by a transformation

$$x_{n(k-1)+i} = X_{ik}, \quad i, k = 1, \dots, n, \tag{8}$$

and defining

$$Q = J \otimes M, \text{ where } J = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix},$$

it is easy to see that (7) can be transformed into the form (6), and the matrix Q has almost block-upper diagonal form.

At the same time, in order to solve the QUBO representation of TSP, it is not enough just to encode the cost function, but we also need to guarantee that X (and hence its vector representation $\vec{x}$) encodes a feasible solution. To do so, one-hot type restrictions are imposed on columns and rows of X, that is,

$$\sum_{i=1}^{n} X_{ij} = \sum_{j=1}^{n} X_{ij} = 1,$$

for all $i, j = 1, \dots, n$. To embed these restrictions into the cost function, quadratic terms are introduced into cost function with (appropriately large) Lagrange coefficients L_{1i}, L_{2i}, $i = 1, \dots, n$. That is, the cost of violating feasibility of the solution (which is zero for a feasible X) is given as

$$\sum_{j=1}^{n} L_{1j} \left(1 - \sum_{i=1}^{n} X_{ij}\right)^2 + \sum_{i=1}^{n} L_{2i} \left(1 - \sum_{j=1}^{n} X_{ij}\right)^2.$$

Taking for simplicity $L_{1i} = L_{2i} = L$ as in `traveling_salesperson_qubo` function of D-Wave `networkx.algorithms` package, noting that the constant $\sum_{j=1}^{n} L_{1j} + \sum_{i=1}^{n} L_{2i} = 2nL$ can be omitted from the optimization function, recalling that (due to binary nature of the unknowns) $X_{ij}^2 = X_{ij}$ and using the transformation (8), after some straightforward algebra, the constraints can be given in QUBO form as

$$\vec{x}^T(-2L\vec{I} + 2L(\vec{U} - \vec{I}))\vec{x},$$

where $\vec{I}$ is the identity matrix and $\vec{U}$ is the matrix of ones. Finally, this gives the QUBO representation of TSP in the form (6) as follows,

$$\vec{x}^T \left(J \otimes M + 2L(\vec{U} - \vec{I}) - 2L\vec{I}\right) \vec{x} \to \min,$$

where, recall, M is the given matrix of distances. Note that at implementation phase, care must be taken, since some QA frameworks may require Q to be upper-triangular.

3. Proposed Approach and its Evaluation

In this section we present a hybrid quantum-classical approach to tackle the TSP problem in QUBO form, both by using QA and VQE techniques. Results of numerical experiments both on the input file from the well-known TSPLIB data source and two small-scale problems related to touristic POI in Karelia Republic are presented.

3.1. Hybrid Approach in Solving TSP in QUBO Form

A representation of the TSP as QUBO problem, as can be seen from the results presented in Section 2, is useful both for the classical (gate-based) QC and for QA. Indeed, solving QUBO problem by VQE may be done by imposing restrictions on the problem Hamiltonian (3) so as to describe interactions only up to pairs of qubits, in a similar way like the Ising form (4) does.

Based on this similarity, it seems fruitful to state the TSP in QUBO form and use either QA or VQE to obtain the (approximate) solution of the optimization problem. This, however, comes at a price of a dramatic increase of the state space and decrease in "density" of feasible solutions. We elaborate more on this in Section 4. To mitigate this effect, we propose the following two-stage hybrid scheme.

At the *first stage*, we define the size $n_q \leq n$ of the subproblem that is to be solved by QC in QUBO form. Fixing the first city (say, city 1) of the tour, the initial path of $n-1-n_q$ cities is enumerated exhaustively. For each such path $x \in \{2, \dots, n\}^{n-1-n_q}$ (having unique cities), we define a submatrix

$$M_x = ||M_{ij}||_{i,j\in\{2,\dots,n\}\setminus x}.$$

At the *second stage*, the solution of a TSP problem with a set of remaining cities $\{2, \dots, n\}\setminus x$ with the costs defined by M_x is obtained by QC. The solution y is then concatenated with the beginning x, and the overall price of the cycle (x, y) is calculated. The result is then obtained after exhaustive enumeration over x is complete. We note that this heuristic is partially inspired by the celebrated Karp's partitioning algorithm, see [38] on the detailed probabilistic analysis of the accuracy of the latter. Note that, due to the nature of QC, the result of the second stage may be suboptimal.

To implement this solution, we used `Qiskit` and `DWave` frameworks for classical QC and QA, respectively. In both cases, at the second stage, the TSP was solved in QUBO form. In the former case, using `qiskit_optimization.applications` library, TSP in QUBO form was augmented with the so-called TwoLocal ansatz, whereas Simultaneous Perturbation Stochstic Approximation `SPSA` optimzier from `qiskit_algorithms.optimizers` library was used to optimize the ansatz. Sampling of VQE was done with the help of `SamplingVQE` function from `qiskit_algorithms` library using the standard Sampler from `qiskit.primitives`. In the latter case, the result of the second stage was obtained by `traveling_salesperson` function from `dwave_networkx.algorithms` library using `SimulatedAnnealingSampler` or `DWaveSampler` from `dwave.samplers` library.

3.2. Experimental Evaluation

In order to validate the proposed approach, a number of numerical experiments were conducted. Those included solving TSP on a few examples; in all cases, the problem had a symmetric distance matrix, and the distances were geographical. The first dataset is `Burma14` from the TSPLIB, which is a standard set of benchmarks and algorithms related to TSP. Two more datasets included distances between POIs for Petrozavodsk city (walking distance) and Karelia Republic (driving/linear distance).

For the experiments in simulation mode, we used Linux-based machine (AMD Ryzen 9 7900X, 16 Gb memory) and Linux-based nodes of the high-performance computing cluster of Karelian Research Center (two Intel Xeon Silver 4215R, 128 Gb memory). Both machines were running Python 3.12, the following versions of libraries were used: `dwave_networkx 0.8.15`, `dwave-samplers 1.4.0`, `qiskit 1.2.0`, `qiskit-algorithms 0.3.0`, `qiskit-optimization 0.6.1`. A small set of experiments was also performed using the trial cloud access to the D-Wave machine.

The first set of benchmarks was used to determine computational capabilities in simulation mode. During these experiments, a *problem of size 8* was solved using *Petrozavodsk* dataset. 8 POIs located within Petrozavodsk city were: "Molecule", "Soldier, Woman and Child" and "Fishers" fountains, Sister-cities gallery, Karelian State Philarmony, Peter the Great monument, Alexander Nevsky Cathedral and National Museum. The walking distances in the dataset were acquired through public maps API.

For the VQE-based solver on Petrozavodsk dataset, the size of QC subproblem for the second stage was set to $n_q = 4$ due to the fact that `SamplingVQE` function required over 1 TB memory for $n_q = 6$, occasionally $n_q = 5$ also produced memory overflow, whereas the TSP problem for 3 cities (for $n_q = 3$) is trivial. The VQE approach reached the globally optimal solution with length 8985 (steps). For QA approach, larger size of QC subproblem can be used (in simulation mode). However, due to heuristic nature of the result, in order to increase the sample set (and hence the quality) $n_q = 4$ was used for QA approach as well. The solution returned for QA after several runs had suboptimal length of 9155. It is important to note that the runtime for QA is dramatically shorter than for VQE (minutes vs. days),

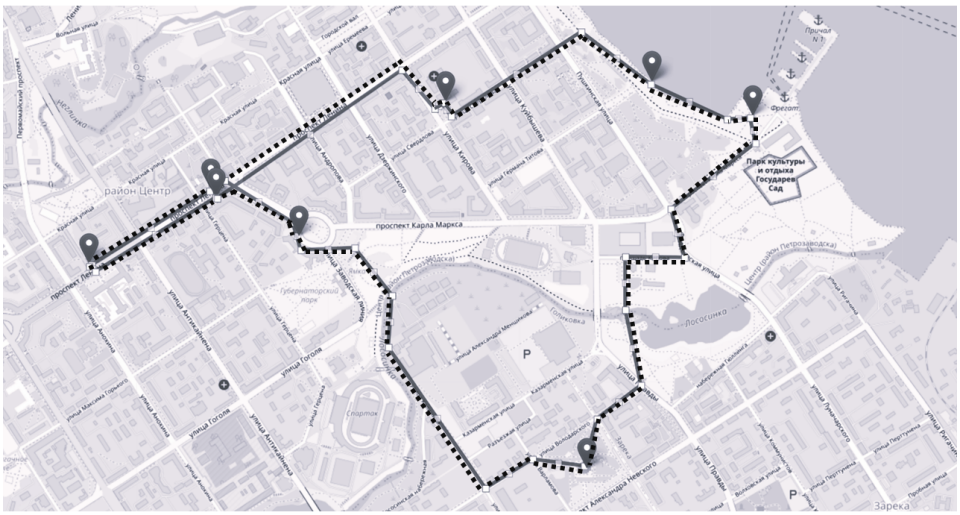

Figure 1. Solutions for the TSP on the *Petrozavodsk* dataset by the two heuristic approaches with $n_q = 4$, dotted line: VQE (tour length 8985 steps), solid line: QA (9155 steps)

which, as we can see, compromises the quality. The best solutions for both approaches obtained in simulation mode are depicted in Figure 1.

The second set of benchmarks was based on the Burma14 dataset. For the VQE approach (with $n_q = 4$), the overall computation time was around 65 hours, whereas for QA in simulation mode it took only several minutes (with $n_q = 8$) to derive an approximate solution. Both approaches performed reasonably well, with the best solution for VQE having tour length 3499 and the best tour for QA in simulation mode having length 3795, compared to the best known result of length 3323 [39]. The best solutions for VQE and QA in simulation mode are depicted in Figure 2.

Running the algorithm on the Burma14 dataset on D-Wave with quantum engines required $n_q \leq 7$ to obtain feasible solutions. Indeed, due to a limited computational time, only 3717 solutions (for the case $n_q = 7$) were derived, and out of those only 140 were feasible, whereas for $n_q = 8$ we did not find any feasible solution out of 935. QA on quantum machine performed slightly worse with tour length 4641. We elaborate more on the reasons for this suboptimality in Section 4.

Due to a reasonable quality of the solutions obtained at higher speed, we used QA approach in simulation mode with $n_q = 4$ to solve the TSP for *Karelia* dataset, where the following 10 natural and cultural POIs were listed: Martsial'nye Vody (Marcial Waters resort), Ruskeala mountain park, Kizhi island, Kiwatsch waterfall, Sortavala city, Syamozero lake, Valaam monastery, Petrozavodsk city, Old Ladoga, and Karelian Zoo. After five runs, the globally optimal solution of length 1676 (kilometers) was obtained, which is depicted in Figure 3. A larger dataset of 18 POIs in Petrozavodsk (including 8 earlier used) was processed by QA approach in simulation mode with $n_q = 12$. The runtime was around 4 hours, and the route including 47488 steps is depicted in Figure 4.

4. Conclusion and Discussion

In this paper we presented a hybrid quantum-classical approach for solving TSP in QUBO form using the VQE and QA as the quantum counterpart, and exhaustive enumeration of the starting path for the

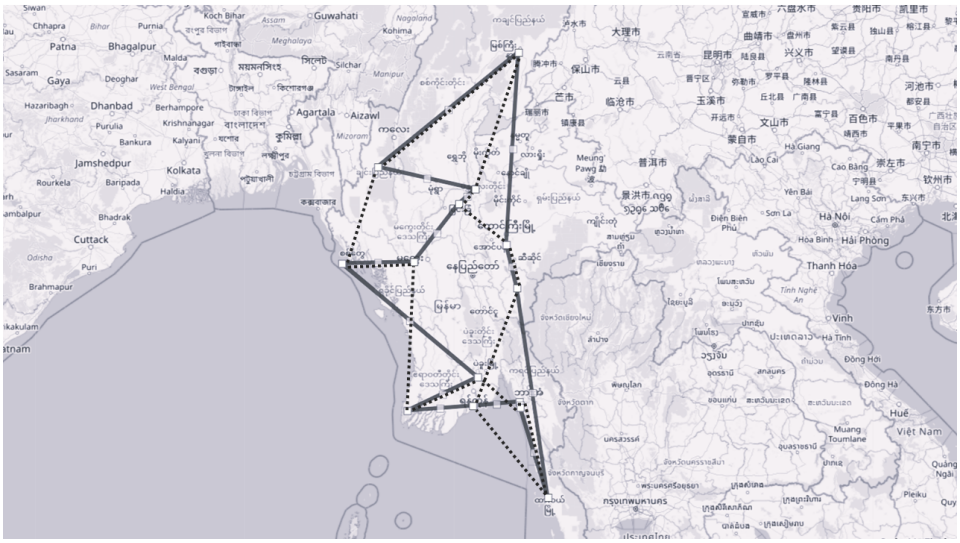

Figure 2. Solutions for the TSP on the Burma14 dataset by the two heuristic approaches, dotted line: VQE ($n_q = 4$, tour length 3499 km), solid line: QA ($n_q = 8$, 3795 km)

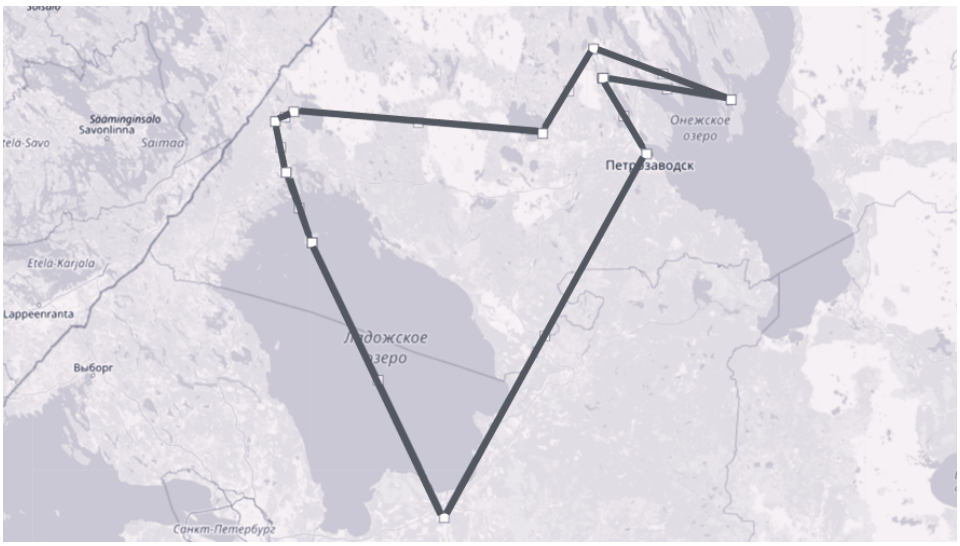

Figure 3. Solutions for the TSP on the *Karelia* dataset (10 POIs) by the QA approach with $n_q = 4$, tour length 1676 km

classical counterpart. The approach performed reasonably well for both QC techniques, although in simulation mode the quality of solutions obtained by VQE was better than those obtained with QA, at a price of dramatically higher computing time.

As for the QA run at the D-Wave machine, there were several problems that allowed us to find feasible solutions only for subproblem size (solved at quantum machine) $n_q \leq 7$. Moreover, for $n_q = 10$ using the `MinorEmbedding`, the cloud was not able to find a quantum engine to run the problem

Figure 4. Solutions for the TSP on the *Petrozavodsk* dataset (18 POIs) by the QA approach with $n_q = 12$, tour length 47488 steps

with. There are several reasons for that. Firstly, as reported in [22], out of m physical qubits only around $\sqrt{m}$ logical are available, thus resulting in about 73 *logical* qubits for the D-Wave computing unit having around 5000 *physical* qubits. Secondly, due to the one-hot encoding (8), a problem of size n requires at least n^2 *logical* qubits. This essentially means that TSP of size n requires around n^4 physical qubits which explains the limitation $n_q \leq 8$ for our case, see also the discussion on the embedding capabilities in [40].

Another problem comes from QUBO encoding (8) is the density of the feasible solutions. It is shown in [18] that such density decreases dramatically for TSP QUBO with increasing size. Indeed, this can be intuitively explained by the fact that the set of n^2-component binary vectors has 2^{n^2} elements, whereas the set of feasible solutions for TSP problem contains only $n!$ (for simplicity, we do not take into account symmetries and fixed starting city). Asymptotic analysis using the celebrated Stirling's formula shows that the ratio of the feasible solutions to the state space of QUBO problem vanishes for large n,

$$\frac{n!}{2^{n^2}} \sim \frac{\sqrt{2\pi n}(n/e)^n}{e^{n^2 \log 2}} \sim e^{n \log n - n + 0.5 \log n - n^2 \log 2} \to 0, \quad n \to \infty.$$

It is rather simple to check that even for the case $n = 6$ the frequency of feasible solution is of order 10^{-8}, see also [18]. This explains the low density of feasible solutions that was evidenced when running QA experiments on hardware with $n_q = 7$, see Section 3.2.

One of the perspective approaches to overcome this "curse of dimensionality" is to find a different encoding for the TSP. In particular, permutation encoding may be promising [18] for the QO approaches that do not rely on Hamiltonian. Other approach is introduced in [23] by converting the TSP problem into a classical Brachistochrone problem and using the single-qubit scheme with

rotations. Other techniques such as Grover adaptive search can also be adopted [19]. However, all those possibilities need careful exploration that seems promising for future research.

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Исследование квантово-классической эвристики для задачи коммивояжера

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Аннотация. В статье разрабатывается и оценивается гибридный квантово-классический эвристический подход к решению задачи коммивояжера. Этот подход использует исчерпывающий перебор начальных путей и оптимизирует оставшуюся часть маршрута с помощью квантовых вычислений. Для обработки на квантовой машине используется либо вариационный квантовый собственный решатель, либо квантовый отжиг. Представлены результаты оценки предложенного подхода на нескольких наборах данных, включая TSPLIB и туристические данные для Петрозаводска и Республики Карелия, как в режиме имитации, так и на соответствующей квантовой машине. Обсуждаются вопросы практической применимости.

Ключевые слова: гибридная квантово-классическая эвристика, задача коммивояжера, вариационный квантовый собственный решатель, квантовый отжиг