Benchmarking Small-Scale Quantum Devices on Computing Graph Edit Distance

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Distance measures provide the foundation for many popular algorithms in Machine Learning and Pattern Recognition. Different notions of distance can be used depending on the types of the data the algorithm is working on. For graph-shaped data, an important notion is the Graph Edit Distance (GED) that measures the degree of (dis)similarity between two graphs in terms of the operations needed to make them identical. As the complexity of computing GED is the same as NP-hard problems, it is reasonable to consider approximate solutions. In this paper we present a comparative study of two quantum approaches to computing GED: quantum annealing and variational quantum algorithms, which refer to the two types of quantum hardware currently available, namely quantum annealer and gate-based quantum computer, respectively. Considering the current state of noisy intermediate-scale quantum computers, we base our study on proof-of-principle tests of the performance of these quantum algorithms.

I. INTRODUCTION

The Graph Edit Distance (GED) [1, 2] represents one of the most common dissimilarity measures used in Pattern Recognition and Image Processing [3, 4]. It has been successfully applied to many real-world tasks such as image recognition, handwritten digit recognition, face and face expression recognition [5–9], and has applications in a variety of areas from computer vision and bioinformatics [10] to cognitive science [11], and hardware security [12]. It has also been used in Machine Learning in order to define more powerful kernels for support vector machines [13], and in combination with kernel machines for pattern recognition [14].

In general, the notion of edit distance (originally introduced for strings and then extended to graphs and general structured data) is given in terms of the operations that must be performed on a pair of data in order to make them identical, and represents a quantitative estimate of their dissimilarity. For example in pattern recognition it measures the strength of the distortions that have to be applied to transform a source pattern into a target pattern. As computing the edit distance is essentially to search for the best (in terms of cost) set of operations in the space of all possible ones, the problem is intrinsically a combinatorial optimization problem and its complexity depends on the structure of the data in the search space. When data are graphs, calculating the edit distance becomes easily inefficient as the complexity of the search space grows exponentially with the number of nodes of the graphs. In fact, the GED problem is an NP-hard optimization problem, which makes exact approaches impossible to use for large graphs. This makes the study of approaches that give near-optimal results in reasonable time an urgent and essential one, also in the light of the practical impact of the GED problem. It is therefore of great importance to discuss and analyze in this context the feasibility of quantum approaches and to compare them on the basis of their performance measured with respect to the existing classical algorithms that have been proposed up to now [2].

The quest for optimization algorithms that can run on noisy intermediate scale quantum (NISQ) computers is a very timely topic, as well as a challenging task [15, 16]. Two main strategies that have been adopted to tackle optimization tasks are Quantum Annealing (QA) [17] and variational quantum algorithms such as Variational Quantum Eigensolver (VQE) [18] and Quantum Approximate Optimization Algorithms (QAOA) [19]. In this paper we analyze the applicability of these two quantum approaches to the problem of computing the edit distance between graphs.

The QA approach can be seen as the quantum analogue of the classical simulated annealing optimization algorithm [20], and essentially consists in using a specific search procedure for finding the state of minimum energy of spin systems studied in statistical mechanics, e.g. the Ising model in a random field [17]. In the quantum case the fluctuations needed to scan the energy landscape are provided by a field that allows quantum tunneling, in contrast to the simulated annealing where the fluctuations are thermal [21].

While QA is based on the adiabatic model of quantum computation, VQE and QAOA are hybrid quantum-classical algorithms implemented on circuit-based quantum computers. This approach has been tested in several proof-of-principle experiments for real-world optimization (e.g. scheduling) problems [22, 23].

Both kinds of approaches share a common physical ground, since they are both implemented by means of a total Hamiltonian that is composed by two non-commuting terms, $H_0$ and $H_1$, such that $[H_0, H_1] = H_0H_1 - H_1H_0 \neq 0$. This Hamiltonian has the form

$$H = (1 - \lambda(t))H_0 + \lambda(t)H_1,$$

where $\lambda(t)$ is a control function that is valued in the interval $[0,1]$ and allows us to switch between the two terms.
In fact, assuming that the computation time is in the interval \([0, \tau]\), one can initialize the system into the ground state of \(H_0\), imposing \(\lambda(0) = 0\), and tune the control parameter till reaching \(\lambda(\tau) = 1\). If the variation of \(\lambda(t)\) is such that the hypotheses of the adiabatic theorem \([24]\) are satisfied, both algorithms can be viewed as prefatory approaches for full adiabatic quantum computation \([25]\). Moreover, the gates composing the QAQC can be seen as a Suzuki-Trotter decomposition \([26]\) of the unitary evolution stemming from a Hamiltonian as defined in (1).

Another common aspect of QA and QAOA is that their performance significantly depends on heuristics for the choice of the annealing schedule and parameter initialization, respectively.

By defining the problem of calculating the GED as a Quadratic Unconstrained Binary Optimization (QUBO) problem, we are able to experiment both on quantum annealers, such as the D-Wave Systems Inc. machines, and on quantum circuits via variational algorithms such as VQE and QAOA. We introduce a QUBO formulation of GED that is similar to the one presented in \([27]\) for the Graph Isomorphism problem, i.e. the computational problem of determining whether two finite graphs are isomorphic. Our formulation exploits the fact that GED can be seen as a quantitative generalization of graph isomorphism, which requires a ‘counting’ phase while checking the nodes/edges in each of the graphs. This allows us to obtain a quantitative answer to the optimization problem rather than just a yes/no answer as in the case of graph isomorphism. This also explains why the GED problem is far more complex than graph isomorphism, for which it was recently shown that the problem is solvable in quasi-polynomial time \([28]\).

In order to assess the relative performance of the classical hardware (through simulated annealing), and the currently available quantum hardware both in its realization as quantum annealer (D-Wave System) and circuit-based quantum computer (IBM Quantum), we construct a benchmark by running the same QUBO formulation on each machine. The importance of such a benchmark is nowadays necessary as a base for assessing the actual power of NISQ devices for real-world problems.

This paper is structured as follows. In Sec. II we introduce the notion of graph edit distance, and in Sec. III its QUBO formulation. Section IV is devoted to the classical approaches developed to compute GED, while in Section V we discuss the methods we employ in our experiments on both quantum annealer and circuit-model quantum computer. In Section VI we present the results of our experiments and provide a comparison among the different strategies. Finally, in Section VII we discuss our results in the light of the currently available technologies and we address some open questions.

II. GRAPH EDIT DISTANCE

A graph \(G = (V, E)\) consists of a finite, non-empty set of vertices \(V\) of cardinality \(|V| = n\), and a set of edges \(E = \{(u, v) \mid u, v \in V\} \subseteq V \times V\) of cardinality \(|E| \leq n^2\). The graph is undirected if each edge is described by an unordered pair of vertices, directed otherwise. In an undirected graph, the number of edges is at most \(n(n+1)/2\) or, by excluding self-loops (edges starting and ending in the same vertex), \(n(n-1)/2\).

Two graphs \(G_1 = (V_1, E_1)\) and \(G_2 = (V_2, E_2)\) are isomorphic, denoted by \(G_1 \cong G_2\), if there exists a bijection \((1\text{-to-1 mapping})\) \(\pi\) between the vertex sets of \(G_1\) and \(G_2\) satisfying the property of edge-preserving \([29]\), i.e. \(\{u, v\} \in E_1 \iff \{\pi(u), \pi(v)\} \in E_2\). The graph isomorphism problem is the problem of establishing the exact matching of two graphs \([29]\). The inexact matching is the more general case where there is a difference between two graphs, and a measure of this difference quantifies ‘how much’ the two graphs are (dis)similar. An important graph similarity measure is the graph edit distance (GED) \([1, 2]\), whose value is the total cost of ‘transforming’ one graph into the other, thus making them isomorphic. Clearly, when two graphs are isomorphic, the GED between them is zero.

The GED problem is a NP-hard optimization problem, i.e. intuitively, it is at least as hard as the hardest problems in NP. This means that it is computationally more expensive than graph isomorphism for which a recent result shows that it is possible to find a solution in quasi-polynomial time \([28]\).

A graph edit operation is a mapping from the set of graphs to itself. The most common edit operations on a graph \(G = (V, E)\) are listed in Table I, where we also specify the part of the graph which they act on (Vertex or Edge set), and the condition of their applicability (Constraint). Specifically, these operations can be performed provided that they do not insert a pre-existing vertex/edge, or delete a non-existing vertex/edge; it must also be guaranteed that before deleting a vertex, each edge starting or ending into that vertex must be deleted.

| Operation          | Vertex set | Edge set | Constraint |
|--------------------|------------|----------|------------|
| Insert node \(v\)  | \(V \cup \{v\}\) | No changes \(v \notin V\) |
| Delete node \(v\)  | \(V \setminus \{v\}\) | No changes \(v \in V, \beta uv \notin E\) |
| Insert edge \(uv\) | \(E \cup \{uv\}\) | No changes \(uv \notin E\) |
| Delete edge \(uv\) | \(E \setminus \{uv\}\) | \(uv \notin E\) |

TABLE I: Main operations composing a graph edit path

A graph edit path \(P\) is a composition of graph edit operations and the number of these operations defines the length, \(\ell(P)\), of the path. The graph edit distance between two graphs \(G_1\) and \(G_2\) can be defined as

\[
\text{GED}(G_1, G_2) = \min_P \{\ell(P) \mid P(G_1) \cong G_2\}. \tag{2}
\]

A more fine-grained definition of GED can be found in
where labelled graphs are considered, so that each graph edit operation might contribute to the graph edit distance with a different weight. For our purpose, it is sufficient to consider the case of unlabelled graphs, which allows us to keep our implementation simpler. In particular, in the calculation of the GED we will assume that each edit operation has cost 1. This implies that the length of an edit path effectively corresponds to the number of operations composing it, which is a reasonable estimate of the complexity of the calculation. An example of calculation of GED is shown in Figure 1.

IV. QUBO FORMULATION OF GED

The graph matching problem can be encoded as a linear optimization problem [31, 32] or a quadratic optimization problem [27, 33]. We show here how the second approach can be extended to inexact graph matching, and precisely to the GED problem. The idea is to reformulate GED as a Quadratic Unconstrained Binary Optimization (QUBO) problem, a class of problems that is well known in multivariate optimization. As the name suggests, a QUBO problem is defined in terms of a quadratic function of binary variables \( x_i \), which is unconstrained or, more precisely, with constraints replaced by penalty terms and encoded within a matrix \( Q \) representing the objective function [34]. The task is to find the value \( x^* \) such that

\[
x^* = \arg \min_x x^T Q x,
\]

where \( x_i \in \{0, 1\} \) for any of the \( n \) entries of \( x \), and \( Q \) is an \( n \times n \) upper triangular real valued matrix with elements \( q_{i,j} \) encoding the data specification.

QUBO problems are NP-hard problems. They share a similar structure and the same computational complexity with Ising models. This similarity allows for an almost immediate implementation of QUBO objective functions into the adiabatic model of quantum computation. To this purpose, a QUBO formulation of many optimisation problems is shown in [35].

In this paper we present a QUBO formulation of the GED problem in analogy with the formulation given in [27] for the graph isomorphism problem.

For the calculation of the GED of two graphs \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \) we shall assume that the number of vertices is the same in both graphs, that is \( |V_1| = |V_2| = n \). This is without loss of generality; in fact, if \( G_1 \) has \( k = |V_1| - |V_2| > 0 \) vertices more than \( G_2 \) we build \( G_2' \) by adding \( k \) isolated vertices to \( G_2 \), then we calculate the GED between \( G_1 \) and \( G_2' \), and finally add \( k \) to the given value for considering the \( k \) insertion node edit operations. The formulation requires \( n^2 \) variables, each denoted by \( x_{i,j} \), with \( x_{i,j} = 1 \) if and only if the \( i \)-th vertex of \( G_1 \) is mapped to the \( j \)-th vertex of \( G_2 \).

We define the dual path of \( P \) as the path, \( \tilde{P} \), where any deletion operation becomes an insertion operation and vice versa. If a bijection \( \pi \) corresponds to a graph edit path \( P \) such that \( P(G_1) \cong G_2 \), we can partition \( P \) in two edit paths \( P_1 \) and \( P_2 \), where \( P_1 \) has only insertion operations and \( P_2 \) only deletion operations. Then

\[
P(G_1) \cong G_2 \text{ if and only if } P_1(G_1) \cong \tilde{P}_2(G_2).
\]

Clearly, \( \ell(P_1) + \ell(P_2) = \ell(P_1) + \ell(\tilde{P}_2) = \ell(P) \). Intuitively, the process is illustrated by the example reported in Figure 2.

Considering the two assumption stated above, we can define the cost of a bijection \( \pi \) as

\[
\text{cost}(\pi) = |E_1 \setminus \pi^{-1}(E_2)| + |E_2 \setminus \pi(E_1)|
\]

where \( \pi(E) = \{\{\pi(i), \pi(j)\} \mid \{i, j\} \in E\} \). For a given bijection \( \pi \), the value of \( \text{cost}(\pi) \) is equal to the number of edges occurring in \( E_1 \) and not in \( E_2 \) plus the number of edges present in \( E_2 \) but not in \( E_1 \). The assumption that the graphs have the same number of vertices guarantees that a bijection exists.

We can now define the GED as:

\[
\text{GED}(G_1, G_2) = \min_{\pi} \text{cost}(\pi).
\]

The QUBO formulation of our problem is composed by two parts: a hard constraint \( Q_h \), whose function is to add a penalty if the solution \( x \) does not represent a bijection (in that case, \( x \) is not a solution for GED) and a soft constraint \( Q_s \), which introduces a penalty for any edge mismatch as in Equation (4).
The soft constraint is

\[
Q_s(\mathbf{x}) = \sum_{\{i,j\} \in E_1} R_{i,j}(\mathbf{x}) + \sum_{\{i',j'\} \in E_2} S_{i',j'}(\mathbf{x}) \tag{7}
\]

with

\[
R_{i,j}(\mathbf{x}) = \sum_{0 \leq i' < n} x_{i,i'} \sum_{0 \leq j' < n} x_{j,j'} (1 - e_{i,j}')
\]

and

\[
S_{i',j'}(\mathbf{x}) = \sum_{0 \leq i' < n} x_{i,i'} \sum_{0 \leq j < n} x_{j,j'} (1 - e_{i,j})
\]

where \(e_{i,j}(k) = 1\) if and only if \(\{i, j\} \in E_k\). The term \(Q_s\) counts how many edges are not preserved by the bijection \(\pi\) implied by \(\mathbf{x}\). In particular, the \(R_{i,j}\) counts the arcs \(\{i, j\}\) in \(G_1\), \(\{\pi(i), \pi(j)\}\) missing in \(G_2\). The \(S_{i',j'}\) terms counts the arcs \(\{i', j'\}\) in \(G_2\), \(\{\pi^{-1}(i'), \pi^{-1}(j')\}\) missing in \(G_1\). We prove now that the term \(\sum_{i,j \in E_1} R_{i,j}(\mathbf{x})\) is equivalent to the term \(|E_1 \setminus \pi^{-1}(E_2)|\):

\[
|E_1 \setminus \pi^{-1}(E_2)| = \sum_{\{ij, \in E_1} (1 - e_{\pi(i), \pi(j)})
\]

\[
= \sum_{\{ij, \in E_1} (x_{i,\pi(i)} x_{j,\pi(j)} (1 - e_{\pi(i), \pi(j)}))
\]

\[
= \sum_{\{ij, \in E_1} \left( \sum_{i' \leq n} x_{i,i'} \sum_{j' \leq n} x_{j,j'} (1 - e_{i',j'}) \right)
\]

\[
= \sum_{\{ij, \in E_1} R_{i,j}(\mathbf{x})
\]

where \(e_{ij}\) is one iff arc \(\{i, j\} \in E_2\). The procedure to identify \(S_{i',j'}\) is equivalent. The complete formulation reads:

\[
Q_{\alpha,\beta}(\mathbf{x}) = \alpha Q_h(\mathbf{x}) + \beta Q_s(\mathbf{x}) \tag{8}
\]

where the choice of parameter \(\alpha, \beta\) decides the weight of each penalty term.

If we set \(\alpha > \beta\) we are guaranteed that all valid solutions, i.e all those having null hard constraint contribution, have lower cost than any non-valid solutions. For graphs of \(n\) vertices, we can choose

\[
\alpha > n^2 \beta, \tag{9}
\]

to ensure that the contribution of the soft constraint \(\beta Q_s(\mathbf{x})\) to the total QUBO problem is always smaller than the contribution of hard one \(\alpha Q_h(\mathbf{x})\). This is because \(n^2\) is the cost of the worst case, i.e when one graph is complete and the other one empty.

If the maximum cardinality of edges is \(|E| = m < n^2\), then Equation (9) becomes \(\alpha > m\beta\).
IV. CLASSICAL AND QUANTUM APPROACHES TO GED

Many classical algorithms for the GED problem exist [30, 36], but all known exact algorithms run in exponential time in the size of its input. The best performing approach uses A* search [37], an algorithm largely used in the popular library NetworkX [38].

Furthermore, many heuristics running in polynomial time in the size of its input, do exist too. The two most common approaches are either based on reduction GED problem to LSAPE (Linear Sum Assignment Problem with Error-Correction [39]) or based on local search.

A different heuristic algorithm is Simulated Annealing (SA) [20]. This probabilistic method minimizes multivariate binary objective functions and can be used to solve QUBO problems. Due to its physical background discussed later in Section V, it can be compared with quantum annealing and quantum computing approaches presented in the following sections. SA can be seen as taking a random walk in the solution space according to a Markov chain parametrized by a temperature parameter $T$ [40].

A. Simulated Annealing

SA works as shown in Algorithm 2 in Appendix A. When starting the algorithm the temperature $T$ is high, and solutions with higher energy are accepted with a probability that follows the Boltzmann distribution. The temperature decreases exponentially and SA has fewer chances to accept high energy solutions. When the temperature is zero, SA works in a gradient-descent fashion and will converge to a local minima. SA is restarted many times (shots), each from a different point of the state space chosen randomly. Finally, the energy of the solution is the single, lowest energy found in all the shots.

B. Quantum annealing

Quantum Annealing (QA) [17, 41] is a meta-heuristic search algorithm that can be used to tackle QUBO problems. This optimization technique finds its roots in a problem mutated by statistical physics, namely the search of the minimum-energy state of a spin system exhibiting a glassy phase [42].

We briefly recall the notation and the physics underlying a class of spin systems, hereafter referred to as Ising-like model. The aim is to clarify the connection between the unconstrained quadratic problems and the search of the ground state of such a class of models.

Let us introduce a classical spin variable $s_i$ that can take values $\pm 1$. The function describing the energy of a system of $N$ interacting spin disposed over a $d$-dimensional discrete lattice is the Hamiltonian:

$$H(s) = - \sum_{\langle i,j \rangle} J_{i,j} s_i s_j - \sum_i h_i s_i$$

(10)

where the $\langle i, j \rangle$ denotes that the sum is over all the first neighboring sites, the $J_{i,j}$ are the couplings between two sites of the lattice and $h_i$ is the external magnetic field acting on each spin.

A quantum version of the Hamiltonian in Equation (10) is obtained replacing suitably the binary variable $s_i$ with an ad hoc Pauli matrix $\sigma^\alpha_i$ with $\alpha = \{x, y, z\}$:

$$H(s) = - \sum_{\langle i,j \rangle} J_{i,j} \sigma^\alpha_i \sigma^\alpha_j - \sum_{i=1}^N h_i \sigma^\alpha_i.$$  

(11)

The problem of finding the ground state of a Hamiltonian describing an Ising Spin Glass is NP-hard and how it relates to the solution of many NP-hard is reported in [43].

The QUBO problem is closely related to the problem of finding the ground state of a Hamiltonian written in terms of spin variable, upon introducing the transformation:

$$x_i \leftrightarrow \frac{1 + \sigma^x_i}{2}$$

(12)

Originally, QA was introduced in [41] as a quantum-inspired, classical algorithm. In contrast to the SA in which the fluctuations to explore the energy landscape are provided by the temperature parameter $T$, quantum annealing uses a transverse field coefficient $\lambda(t)$ called tunneling coefficient that modulates the two terms of the Hamiltonian as in Equation (1). The quantum annealing uses the term $H_0$ usually referred to as the transverse field Hamiltonian that does not commute with the term $H_1$ in which the optimization problem is encoded. The non-commutativity of the two terms provides the fluctuations necessary to exploit the quantum tunneling, and allows us to escape from the local minima by tunneling through hills in the solution landscape [40]. Typically, when the quantum hardware is used, the system is in a superposition of all possible state, with probability amplitudes depending on $H(t)$.

Quantum annealers usually have a certain number of qubits which are connected according to a given topology. Logically, any QUBO variable is mapped to a qubit. Physically, it is possible that two variables linked by a quadratic term $J_{i,j}$ are not connected. This requires us to find a minor embedding [44], thus a mapping of variables to physical qubits such that variables bond by quadratic terms are located to adjacent qubits. If this is not possible, additional qubits are required to represent a single variable. For this reason, to each variable is assigned one logical qubit but this can be mapped to more than one physical qubits. The task of finding a minor embedding consists in searching a minor of the graph associated with the hardware topology which is isomorphic to the one associated to the QUBO problem. Minor embedding is currently solved using heuristics, available on the D-Wave Ocean library.
C. Variational quantum algorithms

We can use the QUBO formulation to solve the GED problem also on gate-based quantum computers, via Variational Hybrid algorithms, which are based on both classical and quantum resources.

We define a parametric quantum circuit (PQC), that depends on an ansatz for the values of the parameters \( \theta = (\theta_1, ..., \theta_M) \). The number of parameters \( M \) depends on the architecture of the circuit and the number of qubits \( n \) (which are equivalent to the variables of the QUBO problem). For example, we can choose rotational gates which naturally depends on a set of rotation angles. As a shorthand we denote the composition of unitary gates composing the PQC by \( U(\theta) \), and the final state of such a circuit by \( U(\theta)|0\rangle^\otimes n = |\Psi(\theta)\rangle \). Then we compute the expectation value of the problem Hamiltonian \( H_C \):

\[
E(\theta) = \langle \Psi(\theta)|H_C|\Psi(\theta)\rangle .
\]

Such Hamiltonian is related to the QUBO formulation by Equation (12). The value \( E(\theta) \) corresponds to the cost function which has to be minimized and the minimization stage is performed classically.

Examples of this kind of algorithms are the variational quantum eigensolver (VQE) [18] and the quantum approximate optimization algorithm (QAOA) [19]. They are mostly used to find the ground state of the Hamiltonian of nonintegrable spin systems [45], which is indeed a minimization task.

The Variational Quantum Eigensolver (VQE) is inspired by the Variational Principle [18] and it has found its most groundbreaking application in chemical-physics simulation [46–48], and depending on the nature of the problem under investigation many different ansätze can be used [49]. The circuit implementing it is shown in Figure 4, and its construction is detailed in Algorithm 3 in Appendix A.

The Quantum Approximate Optimization Algorithm (QAOA) recently introduced in [19, 22, 23, 50] is an application of VQE. The ansatz must respect a particular structure which depends on the Hamiltonian defining the problem.

V. EXPERIMENTAL SETUP

We consider a set of graphs with a number of vertices ranging from three to nine, and we randomly generate the graphs following the procedure explained in [51]. The procedure needs as inputs the number of vertices \( n \) and the probabilities \( p \) of generating edges in the graph. For all the configurations labelled by the number of vertices \( n \in \{3, 4, ..., 9\} \), we generate four graphs \( G_1, G_2, G_3, G_4 \) with edge probabilities \( p_1 = 0.1, p_2 = 0.33, p_3 = 0.66, p_4 = 0.99 \). This means that graph \( G_1 \), generated with probability \( p_1 \), will contain a small number of edges while the graph \( G_4 \) is almost always a complete graph.

We proceed now to compute the GED(\( G_i, G_j \)) with \( i,j = 1,2,3,4 \) for each number \( n \) of vertices. Any computational run has four inputs: the first graph \( G_i \), the second graph \( G_j \) and the parameters \( \alpha, \beta \) of Equation 8. We iterate the runs over all possible pairs of graphs with the same number of vertices, including the pair of a graph with itself. The formulation shown in Equation (8) requires to find some values for parameters \( \alpha, \beta > 0 \). We have tested the efficacy of each choice of parameters by running experiments through SA. We have tried values \( \alpha = 1 \) and \( \beta \in \{1/i \mid i = 1, ..., 10\} \cup \{0.05, 0.01\} \). Since our graphs have at most 9 vertices, by Equation (8) we need \( \beta < \alpha/81 \approx 0.012 \). For our choice of parameters only the case \( \alpha = 1, \beta = 0.01 \) fulfills the condition in Equation (9).

We have run SA 1000 times, and kept the lowest energy solution \( \tilde{\alpha} \). For each run we have calculated the exact GED \( s \) and the approximated one \( \tilde{s} \). As the absolute error \( |s - \tilde{s}| \), grows with the problem size, we have introduced another quantity called the relative difference, which is defined as

\[
\Delta = \begin{cases} 
0, & s = \tilde{s} \\
\frac{s - \tilde{s}}{\max\{s, \tilde{s}\}}, & s \neq \tilde{s}
\end{cases}
\]

and is in the range \([0, 1]\).

The results of our experiments are shown in Table II. They suggest that the best values are those with \( \beta \in [1/4, 1/10] \). Choosing values of \( \alpha \) and \( \beta \), such that the condition (9) is satisfied, ensures the existence of a valid solution, however this is only a sufficient condition. In fact, we have strong numerical evidences that valid solutions exist also for other choices of parameters, for which a constraint linking \( \alpha \) and \( \beta \) is still an open question.
1. The parameter is defined as \( \alpha = 1, \beta \in \{1/i \mid i = 1, \ldots, 10\} \cup \{0.05, 0.01\} \) with respect to the number of vertices \( n \).

### TABLE II: Average relative difference for the experiments

| Values of \( \beta \) | 1/1 | 1/2 | 1/3 | 1/4 | 1/5 | 1/6 | 1/7 | 1/8 | 1/9 | 0.1 | 0.05 | 0.01 |
|-----------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \( 3 \)               | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
| \( 4 \)               | 0.42| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
| \( 5 \)               | 0.52| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06| 0.06|
| \( 6 \)               | 0.53| 0.10| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
| \( 7 \)               | 0.54| 0.32| 0.05| 0.05| 0.05| 0.05| 0.05| 0.05| 0.05| 0.05| 0.05| 0.05|
| \( 8 \)               | 0.48| 0.48| 0.17| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.09| 0.15| 0.09|
| \( 9 \)               | 0.62| 0.50| 0.38| 0.00| 0.00| 0.00| 0.00| 0.00| 0.01| 0.00| 0.09| 0.24|

### A. Classical approaches

The classical heuristics are implemented within the GEDLib library [52] and its Python wrapper GEDLibPy [53].

As discussed in Section IV, one of the classical meta-heuristic considered is the SA. We use the implementation of a simulated annealer provided by D-Wave Ocean SDK [54]. This supplies a uniform platform to run both classical and quantum annealers. A relevant parameter for SA is the number of samples, counting how many times the process returns the solution and restarts.

### B. D-Wave quantum annealers

For our experiments we have used three different, (fully) quantum annealers from hardware company D-Wave: (i) D-Wave 2000Q; (ii) D-Wave Advantage 1.1; (iii) D-Wave Leap Hybrid Solver.

We recall briefly their different characteristics. D-Wave 2000Q has 2041 qubits and uses a Chimera topology having 5974 couplers (physical connections between qubits) [55]. D-Wave Advantage 1.1 has 5436 qubits and uses a Pegasus topology having 37440 couplers. D-Wave Leap Hybrid Solver is not a quantum annealer but a hybrid classical-quantum software whose configurations are fully managed by D-Wave and it is not customizable.

Both D-Wave 2000Q and Advantage allow us to set the configuration of the annealing process, controlled by a parameter \( s \) that grows monotonically from 0 to 1. The parameter is defined as \( s = t/\tau \), where \( \tau \) is the annealing time. For a specified annealing time the evolution proceeds linearly in \( t \).

Any GED computation runs on both machines with the following configurations:

1. **default configuration (DC)**: the annealing time is 20μs, the annealing process proceeds linearly;
2. **configuration Short Time (ST)**: the annealing time is 1μs, the annealing process proceeds linearly;
3. **configuration Long Time (LT)**: the annealing time 500μs, the annealing process proceeds linearly;
4. **configuration Pause Middle (PM)**: annealing schedule is
   - (a) in the first 5μs, \( s \) grows from 0 to 0.45,
   - (b) in the following 94μs, \( s \) remains constant,
   - (c) in the last 1μs, \( s \) grows from 0.45 to 1.

A run is the number of times the annealing is restarted. We have tried each configuration with a different number of runs: ST with \( 10^4 \), DC with both \( 10^3 \) and \( 10^4 \), the others with \( 10^3 \) and we have kept only the lowest energy result.

We expect that the long time configuration might outperform those having shorter annealing time, due to the possibility of exploring the energy landscape widely. However, for longer times decoherence effects due to noise may arise and there is still no direct control of it. This increases the probability of errors.

We also expect the PM configuration to outperform the default configuration, due to the previous evidences suggesting that pausing the schedule in the middle of the process improves the performances [58, 59].

### C. Variational Quantum Algorithms

We used the implementation of VQE and QAOA available on the Qiskit IBM platform [60].

![FIG. 5: Scheme of the QAOA circuit for \( n = 3 \) qubits. The variational ansatz is repeated twice. The number of parameters is fixed to 2p (and does not depend on \( n \)).](image-url)

We briefly recall the construction of the circuit implementing the QAOA as in [19] and in Figure 5 we plot the circuit used to tackle the GED problem. The circuit has as input the state \( |+\rangle^\otimes n \) where \( n \) is the number of variables of the QUBO problem. Such state is obtained from \( |0\rangle^\otimes n \) by applying the Hadamard gate to each qubit. The QAOA ansatz is constructed by repeating \( p \) times two unitary operation \( U_C(\gamma), U_R(\beta) \). The whole ansatz will depend on \( 2p \) parameters \( \gamma_1, \beta_1, \ldots, \gamma_{2p}, \beta_{2p} \in [-\pi, \pi] \). The first unitary operator is defined to be \( U_C(\gamma) = \exp \{-i\gamma H_C\} \) where \( H_C \) is the problem Hamiltonian and depends on our input. The mapping between the QUBO formulation and the Hamiltonian formulation is detailed in Equation (12).
The second unitary operator is called mixing Hamiltonian and is defined to be \( U_B(\beta) = \exp\{-i\beta H_B\} \), where \( H_B = \sum_i \sigma_i^z \). Note that the two Hamiltonians \( H_C, H_B \) must not commute to have not trivial results. The circuit gives as output the state
\[
|\gamma, \beta\rangle = U_B(\beta_p)U_C(\gamma_p) \cdots U_B(\beta_1)U_C(\gamma_1)|+\rangle^{\otimes n}.
\] (15)

The expectation value represents the energy (cost) associated to a particular choice of parameters and must be minimized:
\[
E(\gamma, \beta) = \langle \gamma, \beta | H_C | \gamma, \beta \rangle,
\] (16)
and we stress that the above equation is Equation (13) rewritten for the QAOA case. Finally, the task of the classical optimization is to find the optimal variational parameters such that:
\[
(\gamma^*, \beta^*) = \arg \min_{\gamma, \beta} E(\gamma, \beta)
\] (17)

We perform 2048 runs with randomly initialized parameters, then the classical optimization is performed using the algorithm COBYLA [61]. The construction of QAOA ansatz is detailed in Algorithm 4 in Appendix A.

VI. NUMERICAL RESULTS

Our analysis takes into account the number of vertices \( n \), the hardware and its configurations. We evaluate the performance of each algorithm, illustrated in Appendix A, using three different measures: the average of the relative difference \( \Delta \), the average of success probability, and the average of high-quality probability. The relative difference was defined in Equation (14); the success probability is defined as the percentage of experimental results having \( \Delta = 0 \), and the high-quality probability is defined as the percentage of results having \( \Delta \leq 0.2 \).

All experiments uses the QUBO formulation shown in Equation (8) with parameters \( \alpha = 1, \beta = 0.1 \), which are optimal according to the preliminary analysis in Table II. The choice of these values enforces the hard constraint, maximizing the chances of reaching a valid solution.

We summarized our results in Figures 6-7-8. All the numerical results are reported in Appendix B.

A. Resource usage

The resources exploited by the quantum annealer can give us useful information about the performance of our optimization tasks implemented over different configurations. We focus on the number of logical qubits, i.e. the number of variables of the problem, and physical qubits, i.e. the number of qubits needed to encode the problem by means of the minor embedding procedure. We consider the maximum length of the chain, that is the maximum number of physical qubits needed to encode a single logical qubit, and the chain strength that measures the strength of the interaction between physical qubits belonging to the same chain.

As shown in Table III, the number of logical qubits depends uniquely on the graphs size. The other resources depend on both the topology of the quantum annealer and the quality of the software performing the minor embedding (which is the same for both versions of the hardware). It is evident that D-Wave Advantage produces much smaller embedding; as shorter chains lead to fewer errors, and in fact we obtain more accurate solutions.

Then, we have quantified the resources required for variational algorithms. In Table IV we report the number of qubits which is exactly to the number of variables. Since there is no need of minor embedding, the number of physical qubits corresponds to the number of logical ones. We also report the number of parameters to be trained by the classical optimizer, the depth, i.e the longest path in the circuit, and the size, that is the number of gates.

To have a good estimation of resources, we transpile the circuit in terms of single- qubits rotations \( U_3 \) and CNOT gates.

We immediately see that in general VQE requires much more parameters than QAOA, although it depends mostly on the choice of the variational form. In general, this should lead to longer classical optimization phase.

We were able to run experiments with graphs up to 5
FIG. 6: Comparison of the performance of the many configurations of quantum annealers as function of \( n \) the number of vertices of a pair of graphs. Plots (a)-(b)-(c) compare configurations of D-Wave 2000Q, while (d)-(e)-(f) compares Advantage hardware. Plots (a)-(d) show the relative difference, (b)-(e) the success probability, (c)-(f) the high quality probability.

FIG. 7: Comparison of the performance of SA and the different versions of quantum annealers. (a) shows the average relative difference, (b) shows the success probability, (c) shows the high quality probability.

vertices, since larger instances requires much more computational power for the simulation, which was not available to us. The number of required gates suggests that this approach is not feasible on NISQ hardware due to the low gate fidelity and decoherence errors. Thus, we have performed the calculation on error-free simulators.

B. Comparing Quantum Annealers

We identify the best performing configuration for all the quantum annealers, and then compare their performance with the simulated annealer. Figure 6 compares the different configuration of D-Wave 2000Q and Advantage. For both quantum annealer versions we see that:

- configurations having 10000 runs perform significantly better than configurations with 1000 runs;
- the annealing time that minimizes the relative difference is \( \tau \geq 20\mu s \). Shorter values return inaccurate solutions, and larger values have similar performance but are costly.
- the introduction of the pause in the annealing process does not improve the performance.
In Figure 7 we compare the two versions of the quantum annealer, i.e. the D-Wave 2000Q and the D-Wave Advantage. We compared both versions in their best performing configuration, that is 20µs of annealing time and 10⁸ runs, even though for some values of \( n \) other configurations might slightly outperform this one. The performance of D-Wave Advantage is better than the one of D-Wave 2000Q, but the gap between the two is quite small. This fact contrasts our expectation of much better performance of D-Wave Advantage suggested by its compact minor embedding (less physical qubits used).

Both quantum annealers perform worse than SA. HybridAnnealer D-Wave Leap has performance close to the SA without ever outperforming it. Finally, we have identified which configuration promises the best tradeoff between quality of the solution and total annealing time. This observation is relevant because the cost of using a quantum annealer is proportional to the amount of time used by the machine.

We measure the time to solution (TTS) as

\[
\text{TTS} = \frac{\# \text{ of runs} \times \text{annealing time per run}}{\text{high quality probability}}
\]

for both D-Wave 2000 and D-Wave Advantage. It measures how much time in seconds is required on a quantum annealer to find a high quality solution. The results are shown in Table V. Our experiments show that having the shortest annealing time with a large number of runs gives the best tradeoff in terms of TTS. For \( n = 9 \) vertices no experiment found any high quality solution thus was not possible to estimate such probability.

| \( n \) | D-Wave 2000Q | D-Wave Advantage |
|-------|---------------|------------------|
|       | A  B  C  D  E | A  B  C  D  E    |
| 3     | 0.01 0.20 0.02 0.50 0.10 | 0.01 0.20 0.02 0.50 0.10 |
| 4     | 0.01 0.20 0.02 0.50 0.10 | 0.01 0.20 0.02 0.50 0.10 |
| 5     | 0.01 0.23 0.02 0.57 0.12 | 0.01 0.23 0.02 0.57 0.11 |
| 6     | 0.03 0.25 0.04 0.72 0.14 | 0.01 0.23 0.04 0.57 0.18 |
| 7     | 0.05 0.80 0.08 1.61 0.32 | 0.03 0.80 0.11 2.00 0.32 |
| 8     | 0.17 0.45 0.33 1.14 0.32 | 0.02 0.45 0.17 8.33 1.67 |

TABLE V: Time To Solution for the two hardware configurations, measured in seconds. Legend: \( n \) is the number of vertices, A is 1µs per run \( \times 10k \) runs, B is 20µs per run \( \times 10k \) runs, C is 20µs per run \( \times 1k \) runs, D is 500µs per run \( \times 1k \) runs, E is 100µs per run \( \times 1k \) runs with paused annealing.

C. Comparing variational algorithms

Figure 8 shows the comparison of performance between VQE, QAOA, and SA. Considering the current state of NISQ devices, we have tested variational approach for instances of GED with graphs having at most 5 vertices (thus our circuit uses 25 qubits). In any case, the classical approach leads to much better solutions. In particular, no variational approaches are able to find an exact solution for instances having \( n \geq 4 \) vertices.

Increasing the number of repetitions \( p \) of the layers does not improve the performance. This is in contrast with the surmise that circuits with a higher number of layers (thus more parameters) are more expressive, e.g. for \( n = 5 \) the VQE with \( p = 1 \) (100 parameters) performs better than the VQE with \( p = 3 \) (200 parameters), as in Figure 8.

As a side remark, it turns out that SA is not always the best performing classical approach. Since quantum approaches do not outperform SA, we can state that the nowadays available quantum technologies are not mature enough for the GED problem. The detailed performances of all classical heuristics that we have tested are shown in Appendix B.

VII. CONCLUDING REMARKS

Complex systems are nowadays ubiquitous in science. Very useful models for these systems are typically defined by representing them as graphs, i.e. collections of pairwise connected nodes. The nodes constitute the elementary ‘units’ of the problem, while the edges take into account their interaction. Each edge can also be associated with a label representing some quantitative or qualitative information. This versatility of the graph structures makes them a powerful tool in the most heterogeneous fields of research.

In this paper we have addressed the problem of quantitatively estimating the degree of similarity between a pair of graphs via the Graph Edit Distance. Computing GED is a task that requires the exploration of a space of solutions that is exponential in the size of the input graphs. It is therefore reasonable to consider approximate
approaches to the problem, which are able to achieve acceptable approximations of the exact solution. We have thus investigated whether the resources offered by the quantum hardware currently available are plausible candidates to tackle this task. Our proof-of-principle analysis has had a twofold aim: on one side we have shown how to practically implement the computation of GED on both a quantum annealer and a gate-based quantum computer, and subsequently we have compared the results of running the same GED algorithm on the two types of hardware. Based on our results, the quantum annealer seems to be today a better platform for optimization problems written as QUBO problems. Nevertheless, the development of the gate-based quantum hardware as well as the specific software for optimization algorithms is still in its infancy. It suffers from problems related to the limited amount of physical resources, namely qubits and unitary gates acting for a sufficiently long time [62], and the impossibility (because of the limited resources) of using error-correction schemes as a barrier against noise. Moreover, in order for variational algorithms to work effectively, it is necessary to guess the right encoding of the problem into the parameterized cost function that is evaluated using a quantum computer. This is a challenging task that is crucial for the success of the solution scheme, together with the choice of the best classical optimizers for the parameter training phase.

In this direction, it was recently proposed a Quantum Natural Gradient Descent algorithm [63, 64], which seems to offer enhanced performance by considering statistical information about the quantum circuit such as geometrical methods based on the Quantum Fisher Information [65].

Another seemingly promising strategy is to combine the two approaches that we have studied in this paper, namely using the quantum annealing to get preliminary results that can then be used to initialize a variational algorithm, as shown for the case of the QAOA in [66].

We believe that the algorithms and the benchmarking of quantum annealers and gate-based quantum computers that we have presented in this paper can also be exploited for machine learning tasks. In fact, the algorithms we have devised in our implementations could be profitably incorporated in machine learning algorithms that deal with graph data, to obtain quantum algorithms that are more efficient than the standard classical machine learning strategies.

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S. H. Sack and M. Serbyn, Quantum annealing initialization of the quantum approximate optimization algorithm, Quantum 5, 491 (2021).
In this Appendix we present the algorithms that we have implemented for creating our benchmark. Algorithm 1 is used to construct the QUBO matrix that represents the QUBO formulation of the GED problem.

Algorithm 1: Construct QUBO matrix

Require: $G, H$ graphs having the same number $|n|$ of vertices
Ensure: $Q$ $n \times n$ real matrix

$Q \leftarrow n \times n$ symmetric matrix initialized to zero
$\alpha \leftarrow n^2 + 1$
$\beta \leftarrow 1$

$\forall i \in [0, n)$ do
  $\ell \leftarrow i \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] - \alpha$

$\forall j \in [0, n)$ do
  $\ell \leftarrow j \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] - \alpha$

$\forall i \in [0, n)$ do
  $\ell \leftarrow i \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] + 2\alpha$

$\forall j \in [0, n)$ do
  $\ell \leftarrow j \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] + 2\alpha$

$\forall i, j \in E(G)$ do
  $\ell \leftarrow i \times n + j$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] + \beta$

$\forall i' \in [0, n)$ do
  $\ell \leftarrow i' \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] + \beta$

$\forall j' \in [0, n)$ do
  $\ell \leftarrow j' \times n$
  $Q[\ell, \ell] \leftarrow Q[\ell, \ell] + \beta$

return $Q$

Algorithm 2 represents how the Simulating Annealing procedure we have used works.

Appendix A: Algorithms
Algorithm 2 Simulated annealing

Require: $Q$ QUBO matrix sized $n \times n$
Require: $T_0 > 0$ initial temperature
Require: $\alpha \in (0, 1)$ temperature decrease factor
Require: $S > 0$ number of samples
Ensure: $E$ optimal or sub-optimal cost for minimizing QUBO

1: samples ← empty list
2: energies ← empty list
3: repeat
4:   Generate $x \in \{0, 1\}^n$ randomly
5:   $T \leftarrow T_0$ \hspace{1cm} $\triangleright$ initial temperature
6:   $E \leftarrow x^T Q x$ \hspace{1cm} $\triangleright$ initial energy
7: repeat
8:   $x' \leftarrow$ slightly perturbed $x$
9:   $E' \leftarrow (x')^T Q (x')$
10: $\Delta E \leftarrow E' - E$
11: $r \leftarrow$ random value between 0 and 1
12: if $\Delta E \leq 0$ then
13:   $x \leftarrow x'$ \hspace{1cm} $\triangleright$ accept the solution
14:   $E \leftarrow E'$
15: else if $e^{-(\Delta E)/T} > r$ then
16:   $x \leftarrow x'$ \hspace{1cm} $\triangleright$ accept the solution
17:   $E \leftarrow E'$
18: else
19:   do nothing \hspace{1cm} $\triangleright$ reject solution
20: $T \leftarrow \alpha \cdot T$ \hspace{1cm} $\triangleright$ decrease temperature
21: until $T \approx 0$
22: append $x$ to samples
23: append $E$ to energies
24: $S \leftarrow S - 1$
25: until $S > 0$
26: return samples, energies \hspace{1cm} $\triangleright$ alternately, return min(energies)

Algorithm 3 constructs the parametric quantum circuit needed to run the VQE algorithm.

Algorithm 3 Construct VQE circuit

Require: $p$ repetition of the ansatz
Require: $\theta \in [-\pi, \pi]^{2pn}$ parameters vector
Ensure: Circuit for VQE

1: Create circuit of $n$ qubits
2: for $i \in 1, \ldots, p$ do
3:   for $j \in 1, \ldots, n$ do
4:     Apply gate $R_y(\theta_{2in+2i})$ on $j$-th qubit
5:     Apply gate $R_y(\theta_{2in+2i+1})$ on $j$-th qubit
6:   for $j \in 1, \ldots, n - 1$ do
7:     for $k \in i + 1, \ldots, n$ do
8:       Apply gate $CX$ on $j$-th (control) and $k$-th (target) qubits
9: return circuit

Algorithm 4 constructs the parametric quantum circuit needed to run the QAQA algorithm.
**Algorithm 4 Construct QAOA circuit**

**Require:** $H_C = \sum_{i,j} J_{i,j} \sigma^z_i \sigma^z_j$ defined on $n$ variables  
**Require:** $p$ number of repetition of the Hamiltonians  
**Require:** $\gamma \in [-\pi, \pi]^p$ parameter vector  
**Require:** $\beta \in [-\pi, \pi]^p$ parameter vector  

**Ensure:** Circuit for QAOA  

1: Create circuit of $n$ qubits  
2: for $i \in 1, \ldots, n$ do  
3: Apply gate $H$ on $i$-th qubit  
4: for $i \in 1, \ldots, p$ do  
5: for $J_{i,j} \sigma^z_i \sigma^z_j$ in $H_C$ do  
6: if $i = j$ then  
7: Apply gate $R_Z(\gamma_i J_{i,i})$ on $i,j$-th qubits  
8: else  
9: Apply gate $R_{ZZ}(\gamma_i J_{i,j})$ on $i,j$-th qubits  
10: for $i \in 1, \ldots, n$ do  
11: Apply gate $R_X(\beta_i)$ on $i$-th qubit  
12: return circuit

▷ Circuit starts in state $|0\rangle^\otimes n$  
▷ Circuit evolves in state $|+\rangle^\otimes n$  
▷ Construct $U_C(\gamma_i) = e^{-i\gamma_i H_C}$  
▷ Construct $U_B(\gamma_i) = e^{-i\beta_i H_B}$
Appendix B: Detailed results

Figure 9-11 compares the performances of classical heuristics. All these approaches are detailed explained in [30]. Figure 9 contains the Average relative difference, as defined in Section V by Equation 14.

![Table 9](image)

FIG. 9: Average relative difference (lower is better), Legend: V: number of vertices, B1: Branch, B2: Branch Fast, B3: Branch Tight, B4: Branch Uniform, B5: Branch Compact, P1: Partition, H1: Hybrid, R1: Ring, A1: ANCHOR_AWARE_GED, W1: Walks, I1: IPFP, B6: BIPARTITE, S1: SUBGRAPH, N1: NODE, R2: RING_ML, B7: BIPARTITE_ML, R3: REFINE, B8: BP_BEAM, H2: HED, S2: STAR

Figure 10 contains the Average success probability, as defined in Section VI, which is the percentage of runs having null relative difference over all runs.

![Table 10](image)

FIG. 10: Average success probability (higher is better), Legend: V: number of vertices, B1: Branch, B2: Branch Fast, B3: Branch Tight, B4: Branch Uniform, B5: Branch Compact, P1: Partition, H1: Hybrid, R1: Ring, A1: ANCHOR_AWARE_GED, W1: Walks, I1: IPFP, B6: BIPARTITE, S1: SUBGRAPH, N1: NODE, R2: RING_ML, B7: BIPARTITE_ML, R3: REFINE, B8: BP_BEAM, H2: HED, S2: STAR

Figure 11 contains the Average high-quality probability, as defined in Section VI, which is the percentage of experiments having results with relative difference \( \leq 0.2 \).

![Table 11](image)

FIG. 11: Average high-quality probability (<20%) (higher is better), Legend: V: number of vertices, B1: Branch, B2: Branch Fast, B3: Branch Tight, B4: Branch Uniform, B5: Branch Compact, P1: Partition, H1: Hybrid, R1: Ring, A1: ANCHOR_AWARE_GED, W1: Walks, I1: IPFP, B6: BIPARTITE, S1: SUBGRAPH, N1: NODE, R2: RING_ML, B7: BIPARTITE_ML, R3: REFINE, B8: BP_BEAM, H2: HED, S2: STAR
Figure 12-14 compares the performances of simulated annealing, quantum annealing, variational algorithms. Figure 12 contains the Average relative difference, as defined in Section V by Equation 14.

| V  | SA | D-Wave 2000 | D-Wave Advantage | D-Wave Leap | VQE | QAOA |
|----|----|-------------|------------------|-------------|-----|------|
| 3  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.64 | 0.54 | 0.44 | 0.65 |
| 4  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.86 | 0.76 | 0.88 | 0.91 |
| 5  | 0.06 | 0.20 | 0.06 | 0.06 | 0.09 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.89 | 0.85 | 0.89 | 0.89 |
| 6  | 0.00 | 0.43 | 0.14 | 0.35 | 0.24 | 0.23 | 0.16 | 0.10 | 0.29 | 0.11 | 0.25 | 0.00 | - | - | - |
| 7  | 0.05 | 0.60 | 0.48 | 0.50 | 0.43 | 0.47 | 0.49 | 0.51 | 0.61 | 0.51 | 0.45 | 0.05 | - | - | - |
| 8  | 0.00 | 0.80 | 0.32 | 0.80 | 0.44 | 0.53 | 0.47 | 0.52 | 0.77 | 0.68 | 0.81 | 0.06 | - | - | - |
| 9  | 0.10 | 0.87 | 0.84 | 1.00 | 1.00 | 1.00 | 0.87 | 0.79 | 0.87 | 0.81 | 0.87 | 0.13 | - | - | - |

FIG. 12: Average relative difference (lower is better). Legend: V: number of vertices, D1: annealing 1µs × 10^4 runs, D20: annealing 20µs × 10^4 runs, D21: annealing 20µs × 10^5 runs, D500: annealing 500µs × 10^5 runs, D100: annealing 100µs paused in the middle, ×10^5 runs, p: number of repetition of the variational form

Figure 13 contains the Average success probability, as defined in Section VI, which is the percentage of runs having null relative difference over all runs.

| V  | SA | D-Wave 2000 | D-Wave Advantage | D-Wave Leap | VQE | QAOA |
|----|----|-------------|------------------|-------------|-----|------|
| 3  | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.33 | 0.44 | 0.56 | 0.33 |
| 4  | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.06 | 1.00 | 0.00 | 0.00 |
| 5  | 0.88 | 0.69 | 0.88 | 0.88 | 0.88 | 0.81 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.00 | 0.06 | 0.00 | 0.00 |
| 6  | 1.00 | 0.38 | 0.69 | 0.38 | 0.69 | 0.56 | 0.62 | 0.81 | 0.56 | 0.75 | 0.56 | 1.00 | - | - | - |
| 7  | 0.88 | 0.00 | 0.12 | 0.12 | 0.25 | 0.19 | 0.19 | 0.06 | 0.06 | 0.19 | 0.12 | 0.88 | - | - | - |
| 8  | 1.00 | 0.06 | 0.19 | 0.00 | 0.25 | 0.19 | 0.12 | 0.19 | 0.00 | 0.06 | 0.00 | 0.88 | - | - | - |
| 9  | 0.75 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.69 | - | - | - |

FIG. 13: Average success probability (higher is better). Legend: V: number of vertices, D1: annealing 1µs × 10^4 runs, D20: annealing 20µs × 10^4 runs, D21: annealing 20µs × 10^5 runs, D500: annealing 500µs × 10^5 runs, D100: annealing 100µs paused in the middle, ×10^5 runs, p: number of repetition of the variational form

Figure 14 contains the Average high-quality probability, as defined in Section VI, which is the percentage of experiments having results with relative difference ≤ 0.2.

| V  | SA | D-Wave 2000 | D-Wave Advantage | D-Wave Leap | VQE | QAOA |
|----|----|-------------|------------------|-------------|-----|------|
| 3  | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.33 | 0.44 | 0.56 | 0.33 |
| 4  | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.06 | 1.00 | 0.00 | 0.00 |
| 5  | 0.88 | 0.69 | 0.88 | 0.88 | 0.88 | 0.81 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.88 | 0.00 | 0.06 | 0.00 | 0.00 |
| 6  | 1.00 | 0.38 | 0.81 | 0.50 | 0.69 | 0.69 | 0.75 | 0.88 | 0.56 | 0.88 | 0.56 | 1.00 | - | - | - |
| 7  | 0.88 | 0.19 | 0.25 | 0.25 | 0.31 | 0.31 | 0.31 | 0.25 | 0.19 | 0.25 | 0.31 | 0.88 | - | - | - |
| 8  | 1.00 | 0.06 | 0.44 | 0.06 | 0.44 | 0.31 | 0.44 | 0.44 | 0.12 | 0.06 | 0.06 | 0.88 | - | - | - |
| 9  | 0.94 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.00 | 0.06 | 0.00 | 0.81 | - | - | - |

FIG. 14: Average high quality probability (higher is better). Legend: V: number of vertices, D1: annealing 1µs × 10^4 runs, D20: annealing 20µs × 10^4 runs, D21: annealing 20µs × 10^5 runs, D500: annealing 500µs × 10^5 runs, D100: annealing 100µs paused in the middle, ×10^5 runs, p: number of repetition of the variational form