Transfer learning of optimal QAOA parameters in combinatorial optimization

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Solving combinatorial optimization problems (COPs) is a promising application of quantum computation, with the Quantum Approximate Optimization Algorithm (QAOA) being one of the most studied quantum algorithms for solving them. However, multiple factors make the parameter search of the QAOA a hard optimization problem. In this work, we study transfer learning (TL), a methodology to reuse pre-trained QAOA parameters of one problem instance into different COP instances. To this end, we select small cases of the traveling salesman problem (TSP), the bin packing problem (BPP), the knapsack problem (KP), the weighted maximum cut (MaxCut) problem, the maximal independent set (MIS) problem, and portfolio optimization (PO), and find optimal β and γ parameters for p layers. We compare how well the parameters found for one problem adapt to the others. Among the different problems, BPP is the one that produces the best transferable parameters, maintaining the probability of finding the optimal solution above a quadratic speedup for problem sizes up to 42 qubits and p = 10 layers. Using the BPP parameters, we perform experiments on IonQ Harmony and Aria, Rigetti Aspen-M-3, and IBM Brisbane of MIS instances for up to 18 qubits. The results indicate IonQ Aria yields the best overlap with the ideal probability distribution. Additionally, we show that cross-platform TL is possible using the D-Wave Advantage quantum annealer with the parameters found for BPP. We show an improvement in performance compared to the default protocols for MIS with up to 170 qubits. Our results suggest that there are QAOA parameters that generalize well for different COPs and annealing protocols.

Keywords: QUBO; transfer learning; knapsack; bin packing; portfolio optimization; TSP; maxcut; MIS; quantum optimization; QAOA; combinatorial optimization.

I. INTRODUCTION

Solving COPs is perceived as one of the major application for the near future of quantum computation. There are three main reasons for this. First, COPs can be effectively encoded in Hamiltonians, where the ground state corresponds to the optimal solution of the problem [1, 2]. Second, COPs have practical applications and are hard to solve [3]. Third, quantum algorithms to solve these problems need few resources and can be tested on current state-of-the-art quantum hardware [4–6].

One of the most studied quantum algorithms for solving COPs is QAOA [7]. QAOA consists of p layers, each of which includes the COP cost Hamiltonian encoded in a parametric unitary gate with parameters γ_i and a "mixer" parametric unitary gate with parameters β_i. In this context, the parameters are adjusted to minimize the expectation value of the cost Hamiltonian using a classical optimizer. To some extent, QAOA can be seen as a trotterized quantum annealing protocol where the number of layers p determines the precision of the solution [8]. Over the parametric initialization methods, linear ramp has shown good performance compared with other initialization methods of the QAOA parameters [9]. This method is inspired by an adiabatic evolution, and it gives a first indication that parameters that work on one problem can also be found to work on another problem. The underlying idea of parameter transfer is very promising, as it has been shown that finding parameters for variation quantum algorithms, such as QAOA, is NP-hard [10].

TL has been proposed as a technique to improve the initial guess of QAOA parameters. For instance, in [11], TL of 3-regular graphs in the MaxCut problem was initially introduced as an alternative to do extensive classical optimization for the QAOA parameters. Subsequently, [12] extended this concept to non-isomorphic unweighted graphs in the MaxCut problem and showed optimal QAOA parameter concentration for large graphs. In [13], different properties of random graphs in the MaxCut problem were identified as indicative characteristics of parameter transferability. In [14], numerical evidence supporting an approximation ratio exceeding the worst-case scenario by Goemans-Williamson (GW) was presented for parameters transferred in 3-regular graphs of MaxCut, specifically for $p < 12$. Furthermore, [6] provided indications of TL capabilities in the context of the weighted MaxCut problem. However, the prospects of TL between different COPs have not been systematically investigated to this point.

In this paper, we extend the study of TL capabilities of optimal QAOA parameters across different COPs. To this end, we select random instances of TSP, KP, BPP, PO, MaxCut, and MIS. We first use the Constrained Optimization BY Linear Approximation (COBYLA) [15] optimization method to find β and γ parameters for prob-

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lems with up to 20 qubits. Then, we study the transfer of those parameters to (i) the same COP with up to 42 qubits and (ii) other random instances of completely different COPs. We thereby demonstrate that parameters can not only be transferred to larger instances of the same problem, but also to completely different problems. We use the probability of finding the ground state $probabilty(^{*}x)$ as the performance metric of the TL methodology. From all the COPs studied, BPP is the one that shows best the TL capabilities.

Furthermore, we study the practical TL performance on various quantum technology platforms, namely Aspen-M3 from Rigetti, Harmony and Aria from IonQ, and ibm_brisbane from IBM with problem sizes 8, 14, and 18 qubits. We present solutions of the MIS using QAOA with p=10 and TL from BPP. Our results suggest that even in the 14 qubit case for QAOA with p=10, which corresponds to 640 CNOT gates, a positive net gain of TL may still be observable using IonQ Aria.

Additionally, we explore "cross-platform TL", by transferring the QAOA protocol to a quantum annealing protocol. To this end, we modify the QA protocol of D-Wave Advantage to mimic the QAOA β and γ parameters separately. We study MIS from 100 to 170 qubits and find that the TL protocol of the β parameters performs consistently better than the default D-Wave Advantage annealing protocol.

The rest of the paper is organized as follows. Section II provides a description of the COPs used in this work, the TL methodology, the postprocessing technique for the real hardware implementation to mitigate some of the noise, and a description of the cross-platform TL approach. In Sec. III we present our results and a discussion. Finally, Sec. IV contains our conclusions. The source code for the results shown here can be found at `https://jugit.fz-juelich.de/qip/transfer-learning-QAOA`.

II. TRANSFER LEARNING IN QAOA

In the context of QAOA, we refer to TL as the use of pre-optimized γ_i and β_i for $i = 0, ..., p-1$ parameters on problems that were not used for the optimization. In this methodology, the first step is to find an optimal set of parameters that works well for a specific problem. Then, we test if the optimized parameters work well on different instances of the same and other problems.

We study random instances of TSP, BPP, MIS, KP, PO, and MaxCut using QAOA with $p = 10$. We employ a quantum annealing initialization of the QAOA parameters [9, 16]. To find the minimum of the cost function, COBYLA is employed with a maximum number of iterations given by $\text{max\_iter} = 20N_q p$, where N_q is the number of qubits needed by the problem and p is the number of QAOA layers. Fig. (1) shows the methodology used for (a) the initialization of the γ_i and β_i parameters on the problem selected, (b) the loop of self-optimization where the parameters are updated improving the expectation value of the cost Hamiltonian of the problem, and (c) the TL of the parameters from the problem (BPP) on a new problem – in this case, the MIS. If the TL is successful, the QAOA circuit should sample good solutions for the new problem.

We pick 5 random instances for each problem size. For the TSP, we use instances with 3, 4, 5, and 6 cities (9, 16, 25, and 36 qubits), where the distances between cities are randomly chosen from a normal distribution with mean value 10 and standard deviation 0.1. In the BPP, we consider scenarios involving 3, 4, 5, and 6 items (12, 20, 30, and 42 qubits). The weight of each item is randomly chosen from 1 to 10, and 20 as the maximum weight of the bins. The MaxCut, MIS, KP, and PO problem sizes are 4, 6, 8, 10, 12, 14, 16, 18, 20, 25, 30, 35, 40, and 42. For MaxCut problems, we use randomly weighted edges with weights between 0 and 1 and a probability of having an edge between any two vertices as 70%. In MIS problems, edges between nodes are randomly selected with a 50% probability of having an edge. For KP problems, item values range from 5 to 63, weights from 1 to 20, and maximum weight is set to half of the sum of all weights. Finally, for PO, correlation matrix values are chosen from $[-0.1, 0, 0.1, 0.2]$, asset costs varying between 0.5 and 1.5, and the budget is set to half of the total assets cost. For the inequality constraints in the KP, PO, and BPP, we use the unbalanced penalization approach [17, 18]. Once the QUBO is generated with quadratic penalization terms and translated to the Ising Hamiltonian representation, the Hamiltonian is normalized in all the cases. In Appendix A, we explain in detail the problems and the parameters used in this work.

Mitigation: Hamming distance 1

Our approach uses the Hamming distance 1 strategy as a post-processing technique to reduce errors in real quantum devices. This involves applying a bitflip to each individual position within the output bit-string, to mitigate single qubit bitflips. The computational overhead of this post-processing method is linear, O(NN_q), where N represents the number of samples and N_q is the number of qubits. It is important to note that the success of this method in improving the probability of the ground state relies on the large probability of obtaining the ground state compared to the number of samples used. Also, the error must be low enough to have only a single qubit error in the samples.

Cross-platform TL

In addition to TL between COPs, we also investigate the possibility to apply TL across platforms. In the case of quantum annealing, we want to test the capabilities to transfer the QAOA parameters for solving COPs us-

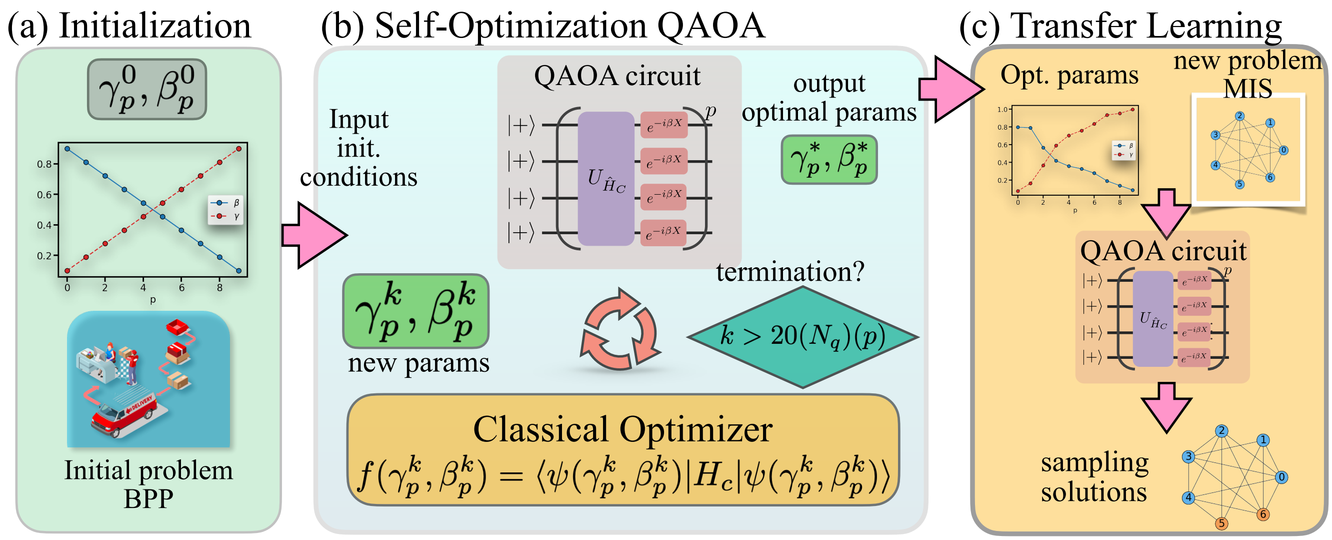

FIG. 1. Example of the TL methodology for transferring the parameters from BPP to MIS. (a) Quantum annealing initialization of the QAOA parameters for $p = 10$ layers using the BPP, (b) self-optimization step using QAOA, (c) final β_i and γ_i parameters transferred to the MIS problem.

ing D-Wave Advantage. The default quantum annealing protocol on D-Wave Advantage, as proposed by Johnson et al. [19], is represented by

$$H(s) = -\frac{A(s)}{2}\sum_i \sigma_x^i + \frac{B(s)}{2} H_c, \tag{1}$$

where $s \in [0, 1]$ is a parameter that represents normalized time, H_c is the problem cost Hamiltonian (see Appendix A for details), $A(s)$ is the annealing protocol associated to the mixer, $B(s)$ is the annealing protocol of the cost Hamiltonian, and σ_x^i is the Pauli-x matrix for qubit i. The default value of s is given by $s = t/t_f$, where t is the instantaneous real time and t_f is the final time. D-Wave Advantage allows modification of the annealing schedule by specifying a maximum of 12 points for the relation $s = f(t)$ between normalized time and instantaneous real time. This flexibility enables us to implement a custom schedule for $A(s)$ or $B(s)$.

We utilize parameters from BPP with 3 items for two modifications of the annealing schedule. Figure 2 shows the two modified annealing schedules for $A(s)$ and $B(s)$, respectively.

III. RESULTS

In this section, we first study, by numerical simulation, TL from one COP to another COP. Using the best parameters, we then perform experiments on various quantum hardware devices. Finally we investigate cross-platform TL, i.e., we learn parameters using a gate-based quantum computing model, and then transfer them to a physical device implementing the quantum annealing model.

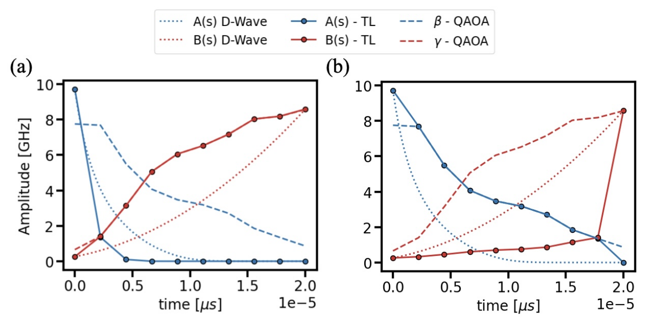

FIG. 2. Example for cross-platform TL parameters on the D-Wave Advantage protocol. (a) TL to the cost Hamiltonian schedule (b) TL to the mixer Hamiltonian schedule. The dotted line represents the default schedule, the solid line is the new schedule with TL applied, and the dashed line reflects the BPP-QAOA schedule. The blue (red) color represents the mixer (cost) Hamiltonian protocol.

Figure 4 shows a comparison between TL from a BPP with 3 items (solid line) vs. self-optimization (dashed line) for the mean value of the optimal *probabilty*($*x$) of the different COPs. Here, each marker represents the mean value over 5 random cases. Self-optimization refers to the optimization of the γ_i and β_i parameters for each specific problem using COBYLA with a maximum number of iterations given by $max\_iter = 20pN_q$, where N_q is the number of qubits and p the number of QAOA layers. The initialization used for all problems was a linear ramp quantum annealing scheme (see Fig. 3 (a)).

The guiding line 'Grover' (black dotted line) indicates a quadratic speedup, i.e., a reduction in the search space to $O(2^{N_q/2})$. The trend for all problems is better than a quadratic speedup with a slight advantage for the self-

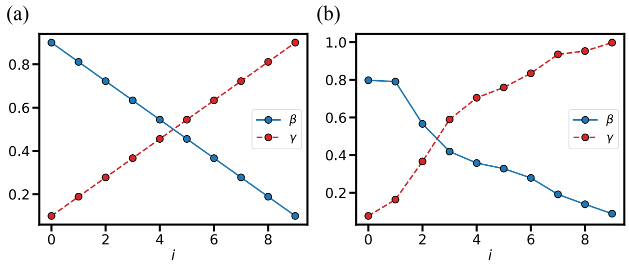

FIG. 3. Example for the QAOA parameter optimizaiton of the BPP. (a) Quantum annealing initialization of the QAOA parameters for $p = 10$ layers, and (b) final β_i and γ_i for $i = 0, ..., p-1$ angles for the BPP with 3 items (12 qubits).

optimization method.

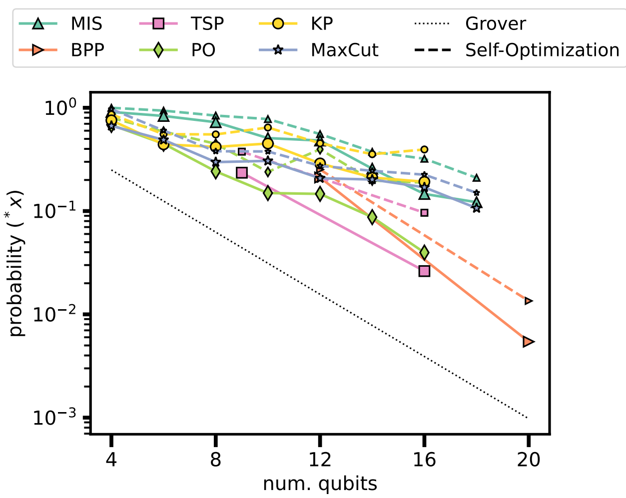

FIG. 4. Comparison between TL and self-optimization for different COPs (see legend). The dashed lines with small markers represent the problems optimized using the procedure in Sec. II, and the solid lines with big markers represent the results of applying TL from the BPP. Grover's quadratic speedup (Grover) is presented as guiding lines.

Figure 5 shows the results of applying TL to larger BPP problems with up to 42 qubits, i.e., we take the resulting 12-qubit parameters and apply the same QAOA schedule to significantly larger problems. The markers represent the mean value based on 5 random cases for each problem size. The solutions in those cases for all the problems are above a quadratic speedup, which is a good indication of the generalization capabilities of the transferred BPP parameters.

Figure 6 shows the results of applying TL from different COPs to (a) the MIS problem and (b) the MaxCut problem on 5 random instances from 4 to 18 qubits. In Fig. 6a, we see that the best performance is obtained by learning parameters from a MIS instance (triangle-up) or a BPP instance (triangle-right). The first can be explained by the fact that different instances of the same problem (MIS) have similar Hamiltonian structures. However, the favourable results for the BPP constitute an interesting empirical observation with no obvious explanation for its generalization capabilities. Figure 6b shows that this observation also holds when transferring to the MaxCut problem, i.e., the best performance is obtained by TL from MaxCut to MaxCut (star) or again from BPP to MaxCut (triangle-right).

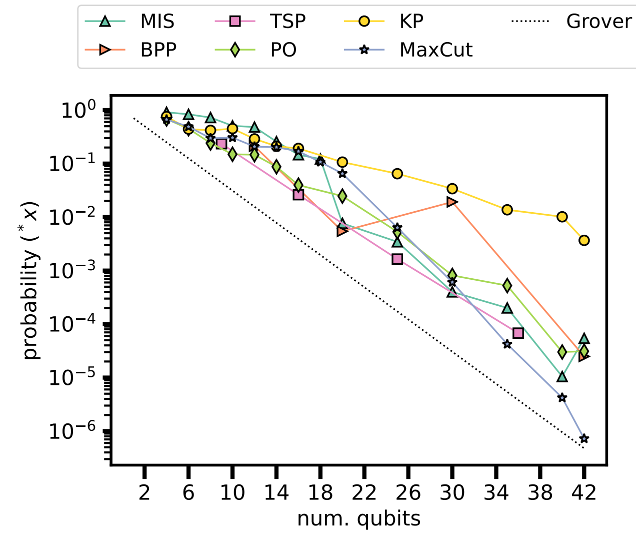

FIG. 5. TL from BPP of 3 items to different COPs. Shown is the mean value of 5 random instances of each problem size of the different COPs. Markers represent the mean value. The guiding line is the same as in Fig. 4.

Solutions on quantum hardware

Next, we show how TL behaves when executing the QAOA algorithm for $p = 10$ on real quantum hardware using the BPP parameters from Fig.3 (b). The problem used is the MIS for random problems with sizes 8, 14, and 18 qubits. The number of samples used are 1000 for the 8 qubit devices, and 5000 for the 14 and 18 qubit devices.

In Fig. (7)-(a), we show results for solving an 8-qubit MIS problem on Rigetti's Aspen-M-3 (2.9%, 27.9%), IBM's Brisbane (4.7% raw, 32.5%), IonQ's Harmony (3%, 21.2%), IonQ's Aria-1 (34.8%, 81.5%), an ideal simulator (89.1%, 94.0%), and random sampling (2.4%, 21%). In this problem, there are 240 CNOT gates on a fully connected device. We can see that at these large circuit depths, Aria is the only device with a distribution resembling the ideal case; all others are similar to a random bitstring generator.

In Fig. (7)-(b), we show results for solving a 14-qubit MIS problem on Rigetti's Aspen-M-3 (0.0%, 0.2%), IBM's Brisbane (0.06%, 0.16%), IonQ's Aria-1 (4.46%, 12.3%), the ideal simulator (19.8%, 30.7%), and a Random Sampler (0%, 0.22%). The probability of connection between different nodes is set to 40%, and 640 CNOT

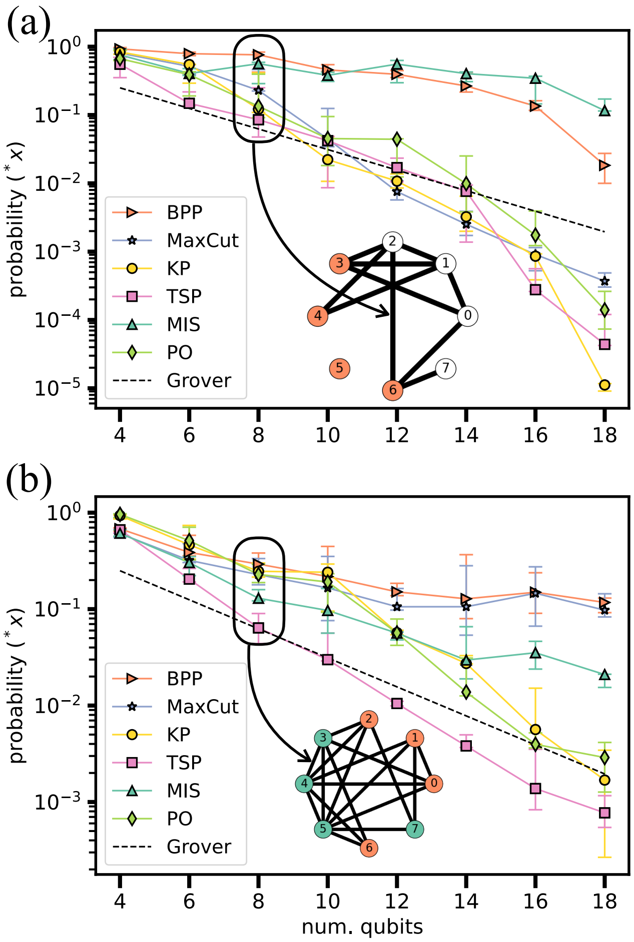

FIG. 6. TL from different COPs to (a) the MIS problem, (b) the MaxCut problem. Using the γ_p and β_p parameters from different COPs, 5 random instance for each problem size of the MIS are solved. Markers represent the median value and error bars represent the Q1 and Q3 quartiles. The insets represent one instance of the respective problem solved using the TL parameters of the other COPs.

gates are applied on a fully connected quantum device. Once again, the results indicate that the probability distribution of the ideal case is very different from the Brisbane and Aspen-M-3 results, whereas for Aria the resemblence with the ideal case is still observable.

Finally, in Fig. (7)-(c) we show results for solving an 18-qubit MIS problem on Rigetti's Aspen-M-3 (0.03%, 0.34%), IBM's Brisbane (0.0%, 0.03%), the ideal simulator (24.1%, 34.8%), and a Random Sampler (0.0%, 0.04%). In this case, the probability of connection between different nodes is 40%, $p = 10$, and the problem requires 1020 CNOT gates on a fully connected device (which corresponds to 3657 ECR gates after transpilation to IBM's Brisbane device). Although IonQ's Aria would also have enough qubits to run this case, testing it was prevented by a limitation in the number of 1 and 2-qubit gates to 950 and 650, respectively. In this case, there is a slight improvement in the Aspen-M-3 result compared to the Random Sampler, but not significantly to conclude that partial information about the probability distribution is recoverable.

Cross-platform TL

In this section, we study cross-platform TL by learning the parameters using a gate-based quantum computer model, and transferring it to a different quantum computing platform, namely a D-Wave Advantage quantum annealer. The results are obtained with 5000 samples for each problem size. Figure (8) shows the TL to the MIS problem for problem sizes 100, 125, 150, 160, and 170 qubits. The green dotted lines are the results using the D-Wave default annealing schedule, the red triangle line is the TL of the mixer Hamiltonian parameters, and the blue circle line is the TL of the cost Hamiltonian parameters. Figure (8)-(a) shows the mean cost with error bars representing the standard deviation of the 5000 sample costs. Figure (8)-(b) shows the minimum cost of the 5000 samples for each problem size. These results show a consistent improvement in the distribution of solutions using TL of the mixer Hamiltonian schedule both in terms of average and minimum value.

IV. CONCLUSIONS

We have presented transfer learning (TL) of QAOA parameters in the context of COP, a methodology that involves using pre-optimized QAOA parameters to solve different COPs. This method therefore does not require extra steps of classical optimization. We show that the BPP has great generalization capabilities, i.e., the parameters for small instances of BPP are good for larger instances of the same problem and effective for instances of other COPs. This is the opposite of what happens with other COPs, where the parameters found do not perform well on other problems.

We test TL using KP, BPP, MIS, MaxCut, TSP, and PO. First, we do self-optimization for these problems, exploring random instances with up to 20 qubits. Then, we select the case with the best performance to find optimal solutions on the other problems. In our case, the parameters used are those of the BPP for 3 items (12 qubits). We use those parameters in different instances of the same and other problems for up to 42 qubits and find that for all of them, the probability of finding the ground state is above the quadratic speedup. This suggests that there are β and γ parameters that generalize well over different COPs.

Next, we show that coherent outputs for problem sizes up to 14 qubits are still present in current quantum technology. We test 3 different instances of the MIS problem with 8, 14, and 18 qubits with the devices used being Rigetti's Aspen-M-3, IBM's Brisbane, IonQ's Harmony and Aria. In the case of 8 qubits, a direct comparison

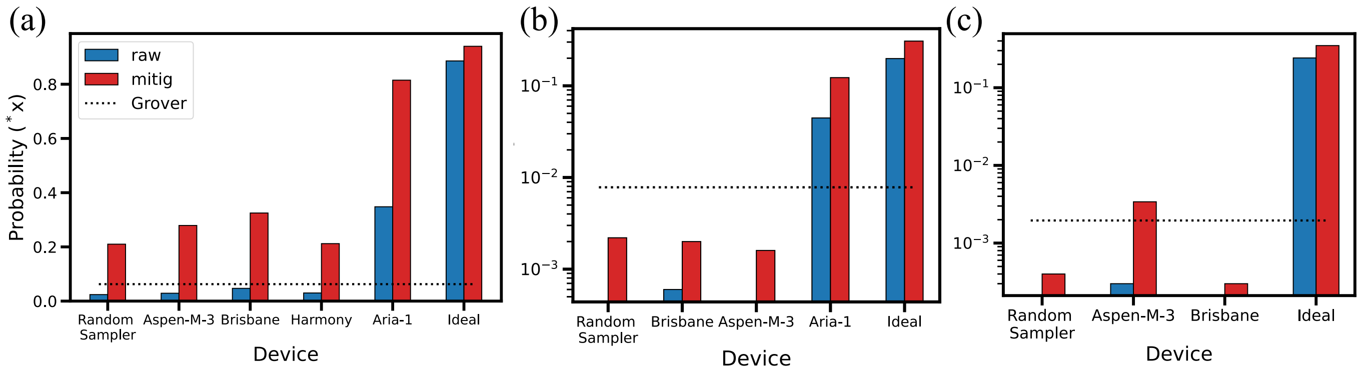

FIG. 7. Success rate to find the optimal solution for different MIS problem size using real devices (a) MIS with 8 qubits with 89.1% of ideal probability (b) MIS with 14 qubits and 19.8% ideal probability (c) MIS with 18 qubits and 24.1% ideal probability. The blue bars represent the raw sampling results using the different devices while the red bars are the percentage of bitstrings with optimal solution and Hamming distance 1 from the optimal solution.

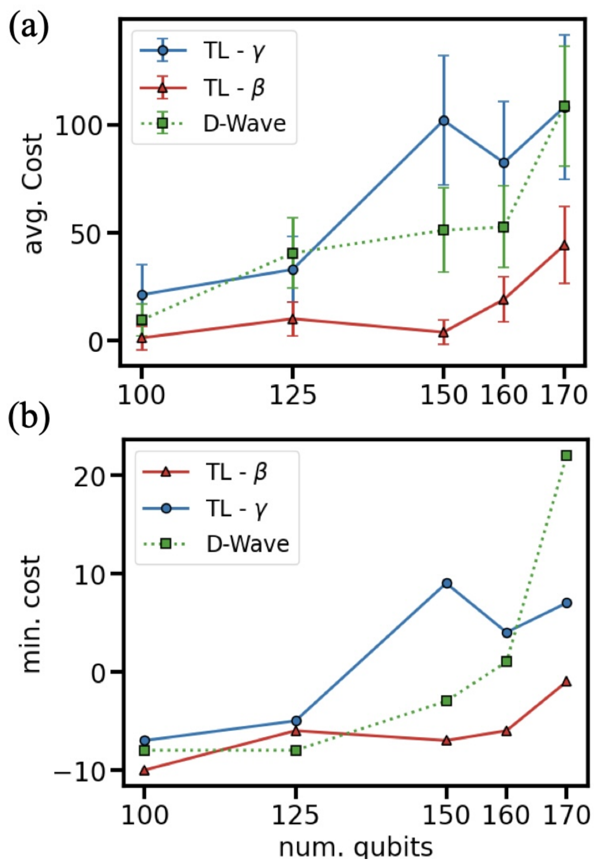

FIG. 8. Cross-platform TL for the MIS using BPP parameters (a) average value using 5000 samples on D-Wave Advantage (b) minimum cost of the 5000 samples.

between the two generations of IonQ technology is possible, Harmony with a success probability of 3.0% and Aria 34.8%. This means an order of magnitude improvement between these two generations of IonQ trapped ions for sampling optimal solutions. There is still room for improvement and benchmarking with this methodology is a promising tool to see the evolution of quantum technology for sampling.

Finally, we show that cross-platform TL is possible. We use D-Wave Advantage to test MIS problems between 100 and 170 qubits using the QAOA parameters of the BPP, Fig. 3. Two cases are tested, one with the modification of the mixer Hamiltonian B(s) and one with the modification of the cost Hamiltonian annealing protocol A(s). We find a consistent improvement in terms of the minimum and average cost using the mixer Hamiltonian modified schedule.

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Appendix A: Supplementary Material

In this section, a description of the different problems used in this work are presented. For each problem, the constraints are encoded using penalization terms. We use squared penalty terms for equality constraints, and the unbalanced penalization approach [17] for inequality constraints.

1. QUBO Formulation

One approach to represent combinatorial optimization problems is through the Quadratic Unconstrained Binary Optimization (QUBO) formulation. The QUBO formulation expresses the problem as a quadratic objective function that depends on binary variables. The objective is to minimize this function by determining the values of the binary variables, subject to certain constraints. Combinatorial problems that can be represented by the QUBO formulation have functions of the form

$$f(\mathbf{x}) = \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} q_{ij} x_i x_j. \tag{A1}$$

Here, n represents the number of variables, $q_{ij} \in \mathbb{R}$ are coefficients associated with the specific problem, and $x_i \in \{0, 1\}$ are the binary variables. It is important to note that in this formulation, $x_i x_i \equiv x_i$ and $q_{ij} = q_{ji}$.

A general form of a combinatorial optimization problem that can be solved using Quantum Processing Units (QPUs) is characterized by a cost function

$$f(\mathbf{x}) = 2 \sum_{i=0}^{n-1} \sum_{j>i} q_{ij} x_i x_j + \sum_{i=0}^{n-1} q_{ii} x_i, \tag{A2}$$

and additionally, linear equality constraints given by

$$\sum_i c_i x_i = C, \quad c_i \in \mathbb{Z}, \tag{A3}$$

and linear inequality constraints given by

$$\sum_i w_i x_i \leq W, \quad w_i \in \mathbb{Z}, \tag{A4}$$

can be added. Here, q_{ij}, c_i, and w_i are parameters of the problem. To transform problems with constraints into the QUBO formulation, the constraints are usually incorporated as penalization terms. The equality constraints are included in the cost function using a penalization term of the form

$$\lambda_0 \left(\sum_i c_i x_i - C \right)^2. \tag{A5}$$

Here, λ_0 is a penalization coefficient that should be chosen appropriately to obtain sufficient solutions that satisfy the equality constraint, and C is a constant value given by the constraint.

For the inequality constraints we use the *unbalanced penalization* [17] encoding which is a heuristic method for including inequality constraints as penalization terms in the QUBO formulation of combinatorial optimization problems. The method has been shown to outperform the slack variables encoding for the TSP, BPP, KP, and in collateral optimization [17, 18, 20]. Starting from Eq.(A4), the method adds a penalization term $\xi(\mathrm{x})$ to the objective function given by

$$\xi(\mathrm{x}) = -\lambda_1 h(\mathrm{x}) + \lambda_2 h(\mathrm{x})^2, \tag{A6}$$

where $h(\mathrm{x}) = W - \sum_i w_i x_i$ and $\lambda_{1,2}$ are penalization coefficients that should be chosen to guarantee that the constraint is fulfilled. The term $\xi(\mathrm{x})$ is unbalanced, meaning that it imposes a larger penalization for negative values of $h(\mathrm{x})$ (i.e., when the constraint is not satisfied) than for positive values. The QUBO formulation using the unbalanced penalization approach is given by

$$\min_x \left(2\sum_{i,j>i} q_{ij}x_ix_j + \sum_i q_{ii}x_i + \lambda_0 \left(\sum_i c_ix_i - C \right)^2 - \lambda_1 h(x) + \lambda_2 h(x)^2 \right). \tag{A7}$$

The parameters for the different problems studied in this work are shown in Table I. In general, this method does not guarantee that the optimal solution is encoded in the ground state of the Ising Hamiltonian. For the probability of the BPP, PO, and KP in Figs. 4 and 5, we choose as optimal solution the ground state of the new Ising Hamiltonian that in the majority of the cases is the optimal solution of the original problem. The last step to represent the QUBO problem as an Ising Hamiltonian is to change the x_i variables to spin variables $z_i \in \{1, -1\}$ by the transformation $x_i = (1 - z_i)/2$. Note that Eq.(A7) can ultimately be rewritten as Eq.(A2) plus a constant value. Hence, Eq.(A2) represented in terms of the Ising model reads

$$H_c(\mathrm{z}) = \sum_{i=0}^{n-1}\sum_{j>i}^{n-1} Q_{ij}z_iz_j + \sum_{i=0}^{n-1} h_iz_i + \text{offset}, \tag{A8}$$

where Q_{ij} and h_i are real coefficients that represent the combinatorial optimization problem, and the offset is a constant value. Since the offset does not affect the location of the optimal solution, it can be left out for the sake of simplicity. In the following subsection a presentation of the different COPs are presented. These problems can be translated into the Ising Hamiltonian representation following the methodology presented in this section. The last step we use to solve the problems using QAOA is to normalize the Hamiltonian by the maximum weight in the Hamiltonian, i.e., $\max\{Q_{ij}, h_i\}$.

TABLE I. Parameters $\lambda_{0,1,2}$ for the TSP, BPP, KP, PO, and MIS used to translate the combinatorial optimization problems into the QUBO representation using the unbalanced penalization approach (Eq. (A7)). For all equality constraints of each problem, we use the same λ_0 and for the inequality constraints the same $\lambda_{1,2}$.

	λ_0	λ_1	λ_2
TSP	23	-	-
BPP	15	4.2	0.4
KP	-	0.96	0.04
PO	-	0.97	0.06
MIS	-	-1	1

2. Combinatorial optimization problems

a. Traveling salesman problem

The TSP is a well-known combinatorial optimization problem that aims to determine the shortest possible route to visit a given set of cities and return to the starting city. This problem has various practical applications, including route planning, circuit board drilling, and DNA sequencing. A QUBO formulation of the TSP can be obtained using a time encoding of the route that the traveller passes on a Hamiltonian cycle [1]. For the asymmetric and symmetric forms, this TSP formulation requires n^2 variables for n cities (we note that in principle, one can reduce this to $(n-1)^2$ variables by fixing the starting point). It needs $2n$ equality constraints and avoids complications associated with sub-tours. The TSP formulation is given by

$$\min \sum_{t=0}^{n-1}\sum_{i=0}^{n-1}\sum_{j\neq i,j=0}^{n-1} c_{ij}x_{i,t}x_{j,t+1}, \tag{A9}$$

subject to the set of constraints,

$$\sum_{i=0}^{n-1} x_{i,t} = 1 \qquad \forall t = 0, ..., n-1, \tag{A10}$$

and

$$\sum_{t=0}^{n-1} x_{i,t} = 1 \qquad \forall i = 0, ..., n-1. \tag{A11}$$

Equation (A10) expresses that at every time t exactly one city is visited, while Eq.(A11) expresses that every city i is visited at exactly one time. For this problem, we use instances with 3, 4, 5, and 6 cities, where the distances between cities c_{ij} are randomly chosen from a normal distribution with mean equal to 10 and standard deviation equal to 0.1.

b. Knapsack Problem

The KP involves selecting a subset of items from a larger set, each with a certain weight w_i and value v_i, in such a way that the total weight does not exceed a given limit, while maximizing the total value. Formally, the cost function is

$$\max \sum_{i=0}^{n-1} v_i x_i, \tag{A12}$$

subject to the single inequality constraint,

$$\sum_{i=0}^{n-1} w_i x_i \leq W, \tag{A13}$$

where $x_i = 1, 0$ indicates that an item is included or not, and W is the maximum weight. We select item values v_i ranging from 5 to 63 randomly, weights w_i from 1 to 20 randomly, and maximum weight $W = \frac{1}{2} \sum_i w_i$.

c. Portfolio Optimization

The goal of PO is to create a balanced portfolio out of a selection of financial assets, which should maximize the future returns, while taking into account the total risk of the investment. The information we have about the assets is their past returns μ_i and the covariances between assets σ_{ij}, with which the problem can be formulated as follows

$$\max \sum_{i=0}^{n-1} \mu_i x_i - q \sum_{i=0}^{n-1} \sigma_{ij} x_i x_j, \tag{A14}$$

subject to the inequality constraint

$$\sum_{i=0}^{n-1} c_i x_i \leq B, \tag{A15}$$

where (similar to the KP), the x_i indicate whether an asset is selected as part of the portfolio or not, and B is the total budget. The factor q controls how much risk is taken. If it is small, the second term in Eq.(A14) becomes negligible and the returns μ_i will be dominant in determining the optimal solutions. In the main text, problem sizes ranging from 4 to 42 are presented. The values of the expected return μ_i are randomly chosen between 0 and 1. The correlation matrix $\sigma_{i,j}$ is selected randomly from the set $[-0.1, 0, 0.1, 0.2]$. Asset costs c_i are randomly chosen between 0.5 and 1.5. The budget is set as $B = \frac{1}{2} \sum_i c_i$.

d. Maximal Independent Set

The MIS problem asks to find the largest subset of vertices of a graph, such that no two vertices in the subset are adjacent. This subset is then called independent. Formally, for an undirected graph $G = (V, E)$, the problem formulation is

$$\max \sum_{v \in V} x_v, \tag{A16}$$

subject to

$$x_u + x_v \leq 1 \qquad \forall (u,v) \in E, \tag{A17}$$

where the binary variable x_v determines whether a vertex is included in the subset or not. We select problem sizes between 4 and 42 qubits and probability of having an edge between nodes of 50%. The constraints in this cases are added to the QUBO formulation as $2x_i x_j$ if an edge is present.

e. Bin Packing Problem

The BPP involves the efficient packing of a collection of items into the minimum number of bins, where each item has an associated weight and the bins have a maximum weight capacity. This problem finds applications in various real-world scenarios, including truck loading with weight restrictions [21], container scheduling [22], FPGA chip design [23] among others. The BPP is classified as an NP-hard problem due to its computational complexity. The problem can be formulated as follows, minimize the total number of bins used given by the objective function

$$\min \sum_{j=0}^{m-1} y_j, \tag{A18}$$

subject to the following constraints. Each bin's weight capacity should not be exceeded

$$\sum_{i=0}^{n-1} w_i x_{ij} \leq W y_j \quad \forall j = 0, ..., m-1, \tag{A19}$$

and each item can only be assigned to one bin

$$\sum_{j=0}^{m-1} x_{ij} = 1 \quad \forall i = 0, ..., n-1. \tag{A20}$$

Binary variables indicating item-bin assignments and bin utilization

$$x_{ij} \in 0,1 \quad \forall i = 0, .., n-1 \quad \forall j = 0, .., m-1, \tag{A21}$$

$$y_j \in 0,1 \quad \forall j = 0, .., m-1. \tag{A22}$$

In the above equations, n represents the number of items (nodes), m represents the number of bins, w_i is the weight of the i-th item, W denotes the maximum weight capacity of each bin, and x_{ij} and y_j are binary variables representing the presence of item i in bin j and the use of bin j, respectively. The objective function in Eq.(A18) aims to minimize the number of bins used, while Eq.(A19) enforces the constraint on bin weight capacity. Eq.(A20) ensures that each item is assigned to only one bin, and Eqs.(A21) and (A22) define the binary nature of variables x_{ij} and y_j. In the main text, we consider scenarios involving 3, 4, 5, and 6 items. The weight of each item w_i is randomly chosen from 1 to 10, and 20 as the maximum weight W of the bins. The Lagrange multipliers $\lambda_{0,1,2}$ in Eq.(A7) for this problem are 15, 4.2, 0.4, respectively.

f. Maximum Cut

The MaxCut problem involves determining the partition of the vertices in an undirected graph such that the total weight of the edges between the two sets is maximized. For an undirected graph $G = (V, E)$, the problem is formulated as

$$\max \sum_{(i,j)\in E} w_{ij}(x_i + x_j - 2x_i x_j), \tag{A23}$$

where w_{ij} represents the weight of the edge between vertices i and j, and x_i and x_j are binary variables that determine the partition of vertices. The goal is to maximize the sum of edge weights over all edges in the cut. The binary variables x_i and x_j take values of 0 or 1, indicating the membership of vertices in different sets of the partition. If x_i and x_j are different, the edge contributes to the objective function.