Quantum Optimization for the Graph Coloring Problem with Space-Efficient Embedding

Abstract—Current quantum computing devices have different strengths and weaknesses depending on their architectures. This means that flexible approaches to circuit design are necessary. We address this task by introducing a novel space-efficient quantum optimization algorithm for the graph coloring problem. Our circuits are deeper than the ones of the standard approach. However, the number of required qubits is exponentially reduced in the number of colors. We present extensive numerical simulations demonstrating the performance of our approach. Furthermore, to explore currently available alternatives, we also perform a study of random graph coloring on a quantum annealer to test the limiting factors of that approach, too.

Index Terms—quantum computation, QAOA, graph coloring, quantum annealing, quantum circuits

I. INTRODUCTION

Quantum computers are expected to offer speedups over classical computers in solving various computational tasks. The recent demonstration of quantum computational advantage by Google researchers [1] further strengthened the case for the practical potential of quantum computation. However, despite the many promising results, the limitations of the near-term Noisy Intermediate-Scale Quantum (NISQ) devices has also been highlighted [2]. Currently, various architectures and physical realizations are being considered for quantum processors, e.g., superconducting qubits [3]–[5], ion-trap-based systems [6], [7], integrated quantum optics [8], [9].

The different quantum hardware implementations have different strengths and weaknesses. For example, scaling up the number of qubits in superconducting architectures is easier than in ion trap systems, while the latter gives rise to deeper circuits. Due to these different features, there has been an intensive discussion about how to define a suitable metric to quantify a quantum processor’s performance, one measure being the so-called quantum volume [10]. Consequently, the challenge to compile large problems into programs (circuits) that minimize the number of qubits and/or the circuit depth has become of central importance in the quantum computing community. Our paper addresses this challenge by introducing a new space-efficient embedding of the graph coloring problem. By applying this method as an input for the Quantum Approximate Optimization Algorithm [11], we obtain a deeper circuit but the number of required qubits (circuit width) is exponentially reduced in the number of colors compared to the standard quadratic binary embedding method. Our numerical studies also indicates that the increase of the depth might not be that significant for larger system sizes, as one needs less levels in the space-efficient embedded version. Moreover, the number of iterations to reach nearly optimal parameters is also significantly decreased compared to the standard version.

The paper is organized as follows. In the next section, graph coloring as a QUBO problem is reviewed. In Sec. III, we present our novel space-efficient embedding method for the graph coloring problem. In order to test the current quantum hardware’s performance on graph coloring, Sec. IV is devoted to experimenting on D-Wave’s quantum annealer, covering a wide range of Erdős-Rényi random graph instances. In Sec. V, we outline the Quantum Approximate Optimization Algorithm (QAOA). We also present numerical simulation results for both the standard and the space-efficient QAOA methods applied to graph coloring problems of different graphs. Finally, Sec. VI summarizes our findings.

II. GRAPH COLORING AND ITS REFORMULATION AS A QUBO PROBLEM

In this section, we shortly review the basics of the coloring problem and its standard formulation as a Quadratic Unconstrained Binary Optimization (QUBO) problem, we introduce the relevant notations and relate our results to previous studies.
A. Graph Coloring

Graph coloring is a way of labeling the vertices of a graph with colors such that no two adjacent vertices are assigned the same color. A coloring using at most $k$ different labels is called a $k$-coloring, and the smallest number of colors needed to color a graph $G$ is called its chromatic number.

Graph coloring has many applications in a wide range of industrial and scientific fields, such as social networks [12], telecommunication [13], and compiler theory [14]. Due to this, it has been in the focus of attention of researchers in computer science and operations research. Although graph coloring, in general, is NP-hard [15], the hardness of a coloring problem is highly dependent on the graph structure and number of colors, and for some special cases, there exists polynomial time exact solvers. For the general case, approximate solution can be achieved by using heuristic algorithms such as Tabu search [16] and Simulated Annealing [17].

B. Graph Coloring as a QUBO Problem

QUBO is a standard model in optimization theory that is frequently used in quantum computing as it can serve as an input for algorithms like the Quantum Approximate Optimization Algorithm (QAOA) [11] or Quantum Annealing (QA) [19]. The general form of QUBO problems is the minimization of $f: \{0, 1\}^n \rightarrow \mathbb{R}$, the pseudo-Boolean objective function of the following form:

$$
\text{minimize } f(x) = x^T Q x = \sum_{i,j=1}^{N} Q_{ij} x_i x_j ,
$$

$$
\text{subject to } \sum_{i \in \{1, \ldots, n\}} x_i = k,\quad x_i \in \{0, 1\},
$$

where $Q$ is a real symmetric matrix, $f$ is often called the cost function and $x^*$ is referred to as a solution bit string or a global minimizer of $f$.

Such a QUBO problem is equivalent to finding the ground-state energy and configurations of the following $N$-qubit Ising Hamiltonian [20]:

$$
H = \sum_{i,j=1}^{N} Q_{ij} (\mathbb{1} - Z_i)(\mathbb{1} - Z_j) ,
$$

where $Z_k$ denotes the operator that acts as the Pauli-$Z$ gate on the $k$th qubit and as identity on the other qubits.

The coloring problem, similarly to several other families of NP-complete problems, can be naturally formulated as a QUBO problem. The QUBO description of the $k$-coloring problem for a graph with $n$ nodes uses $N = n \cdot k$ number of bits. The bits $x_{v,i}$ in this formulation have double labels $(v, i)$, where $v \in \{1, \ldots, n\}$ labels the vertices and $i \in \{1, \ldots, k\}$ labels the colors. One uses a one-hot encoding, i.e., if vertex $v$ is assigned the color $j$ we set $x_{v,j} = 1$ and for all $i \neq j$ we set $x_{v,i} = 0$. To ensure that the solution of the QUBO will satisfy such a one-hot encoding requirement, one employs a penalty term for each vertex $v$ of the form $(1 - \sum_{i=1}^{k} x_{v,i})^2$. Next, for all pairs $(v, w)$ of neighboring sites, one penalizes the same-color assignments by the term $\sum_{i=1}^{k} x_{v,i} x_{w,i}$. Thus, in total, the cost function for the $k$-coloring of a graph with $n$ nodes and adjacency matrix $A$ can be written as follows:

$$
f(x) = C \sum_{v=1}^{n} \left(1 - \sum_{i=1}^{k} x_{v,i}\right)^2 + D \sum_{v,w=1}^{n} \sum_{i=1}^{k} A_{vw} x_{v,i} x_{w,i},
$$

where $C$ and $D$ can be arbitrary positive numbers. The corresponding Ising model is thus:

$$
H = C \sum_{v=1}^{n} \left(2(1 - \sum_{i=1}^{k} (\mathbb{1} - Z_{v,i}))^2 + D \sum_{v,w=1}^{n} \sum_{i=1}^{k} A_{vw} (\mathbb{1} - Z_{v,i})(\mathbb{1} - Z_{w,i})\right).
$$

III. SPACE-EFFICIENT GRAPH COLORING EMBEDDING

We now introduce a method to map the $k$-coloring problem to the ground-state problem of a Hamiltonian using only $n \lceil \log k \rceil$ instead of $nk$ qubits that are required by the standard QUBO method. This embedding will be used to set up a space-efficient QAOA method for coloring in Section IV.

We will first describe the embedding of the 4-coloring problem of an $n$-vertex graph into a 2$n$-bit Hamiltonian optimization problem. The four colors will be encoded by 2 bits (00, 01, 10, 11). To each vertex $v$, we assign two bits $b_{v,1}$ and $b_{v,2}$, and the bit-string $(b_{v,1}, b_{v,2})$ encodes the color that we assign to vertex $v$. To ensure that two neighboring vertices do not have the same color, we introduce the penalty term

$$
b_{v,1} b_{w,1} b_{v,2} b_{w,2} + (1 - b_{v,1}) (1 - b_{v,1}) (1 - b_{w,1}) (1 - b_{w,2}),
$$

since this term is only zero if the colors assigned to $v$ and $w$ differ. Thus, in the case of a graph with adjacency matrix $A$, the 4-coloring problem translates to the ground-state problem of the Hamiltonian

$$
H = \sum_{v,w=1}^{n} \sum_{i=1}^{n} A_{vw} \left(Z_{v,1} Z_{w,1} Z_{v,2} Z_{w,2} + Z_{v,1} Z_{w,2} Z_{v,2} Z_{w,1} + Z_{v,2} Z_{w,1} + Z_{v,2} Z_{w,2}\right) + c_1 \mathbb{1},
$$

where the irrelevant constant term in the last line can be omitted.
graph coloring problem can be embedded into the ground state problem of the \((n \log k)\)-qubit Hamiltonian

\[
H = \sum_{v,w=1}^{n} A_{vw} \sum_{\ell=1}^{m} \prod_{a \in \{0,1\}} (1 + (-1)^{a_{v,\ell}} Z_{v,\ell})(1 + (-1)^{a_{w,\ell}} Z_{w,\ell}),
\]

(5)
since the computational basis state \(\otimes_{v,j}|b_{v,j}\rangle\) is a ground state (in this case a 0-energy state) of \(H\) iff the bitstrings \(b_{v,j}\) provide a proper coloring of the graph.

If the number of colors \(k\) is not a power of 2, i.e., \(2^{m-1} < k < 2^m\), then we again label the colors with \(m\)-long bitstrings \((b_1, b_2, \ldots, b_m)\), but only those are allowed for which \(\sum_{j=1}^{m} 2^{k-j} b_j < k\) is satisfied. One can consistently add new terms to the Hamiltonian such that the non-allowed bit-strings are penalized, as we show in \([21]\). In particular, for the case of \(k = 3\) colors, we will have a Hamiltonian that is a sum of two terms: the first being the same Hamiltonian as for the problems of 4 colors, \(E_{3}\), and the second term being \(\sum_{v=1}^{n} (1-Z_{v,1})(1-Z_{v,2})\) that penalizes the non-allowed \((b_{v,1}, b_{v,2}) = (1, 1)\) assignments, while giving zero for the allowed \((b_{v,1}, b_{v,2})\) values.

IV. QUANTUM ANNEALER EXPERIMENTS

In this section, to explore current possibilities of quantum hardware, we present a study to uncover the main limiting factors of graph coloring solved with quantum annealer (QA) devices. We created a series of experiments to be performed with the currently available D-Wave QA hardware.

A. Quantum Annealing for the Coloring Problem

When graph coloring is reformulated as a QUBO problem, as discussed in Sec. [1] its cost function is equivalent to an Ising model and its global optimum can be approximated by QA \([18], [19]\). We test the limit of this approach using the commercially available quantum annealer, the D-Wave 2000Q which implements a programmable Ising spin network using superconducting flux qubits \([22]\).

The D-Wave 2000Q QPU quantum annealer has at most 2048 available qubits, and has a C16 Chimera topology (the working graph) consisting of a 16 \(\times\) 16 matrix of 8-qubit bipartite graphs. To create a bridge between logical and physical representation of qubits, a technique called minor-embedding maps logical qubits to physical ones.

Since minor-embedding is an NP-hard problem, heuristic algorithms can be employed to find an embedding of the coloring problems \([22]\). While theoretically any graph with \(n\) nodes can be minor-embedded into a Chimera graph with \(O(n^2)\) nodes \([24]\), several studies of minor-embedding algorithms suggest that, the set of completely embeddable problems is also limited by the effectiveness of the minor-embedding algorithm \([25], [27]\).

Another problem with the minor embedding is that it connects physical qubits otherwise not connected (due to the sparse Chimera structure), creating \(chains\) of physical qubits that tend to grow very long in case of large problem complexity. We measured how the lengths of these physical qubit chains, created by automated minor-embedding, are effected by the number of nodes and colors and the edge probability of the ER graphs affect the lengths of these physical qubit chains, created by automated minor-embedding. Fig. [1] summarizes the successful embeddings for random graphs, as the result of more than 50000 embedding trials.

B. Coloring Experiments with Random Graphs

To test the quantum annealing algorithm for the \(k\)-coloring problem, we used \(\text{Erdős-Rényi}\) random graphs generated according to the \(G(n, p)\) model, i.e., a graph of \(n\) nodes is generated by randomly including each edge with probability \(p\). The \textit{average connectivity} \(c\) of such graphs is given by \(c = pn\).

It is known that there exists a threshold of average graph connectivity above which the graph cannot be colored with \(k\) colors, the threshold grows asymptotically as \(2k \ln k\) \([28]\). For smaller number of colors there are different ways to estimate this threshold. For example, it was shown by a heuristic local search algorithm \([29]\), that is based on Potts spin glass model representation of graph coloring, that one can find 3, 4, and 5-colorings of random graphs with at most 4.69, 8.9, 13.69 average connectivity, respectively. Our dataset consisted of quantum anneals with more connected graphs that could be optimally colored, however, we paid attention to these limits in our evaluation.
C. Experimental Results and Findings

To measure the problem size, we use the term problem volume, which is simply the multiplication of the problem parameters \(v = npk\). On small scales \((v < 7)\), the D-Wave annealer was able to solve every single problem, including the evaluation graph coloring problems mentioned in Sec. [V]. As the logical connectivity of the problem graph increased, the quality of the solutions started to degrade, indicated by slowly arising coloring errors. These errors formed either as missing node colors, or as pairs of adjacent nodes sharing the same colors. The summation of these errors is shown in Fig. 2.

While the D-Wave machine performed well on the smaller problems, the illustrations show how it failed to solve most of the complex problems due to the sparse connectivity of the working graph. However, we believe, that by using custom embedding procedures, or by fine-tuning the parameters of the solver, these results could improve significantly [30]. The biggest random graph problem (27 nodes) that we could solve on D-Wave is depicted in Fig. 3.

It is worth mentioning, that we were able to solve more than 90% of the embeddable problems perfectly with simple Tabu-search algorithm, with the search run-times restricted to a couple of seconds. For this purpose, we used the algorithms provided by D-Waves’ Hybrid framework.

We also ran the problems on the D-Wave Leap’s Hybrid Solver, which is a cloud-based quantum-classical solver. The hybrid solver managed to solve all (except one) of the hardest problems (ranked by the embedding chain lengths) with computing time limited to 3 seconds (which is the minimum time limit, for this solver). It should be noted, however, that the QPU time per run used by the hybrid solver exceeded twice the time that was required for a pure QPU sampling run.

V. SIMULATIONS OF THE STANDARD AND SPACE-EFFICIENT QAOA FOR GRAPH COLORING

In this section, we present results for the simulation of the newly introduced space-efficient QAOA algorithm for the coloring problem and compare it to the standard approach that uses the QUBO embedding. We refer to the evaluation graphs shown in Fig. 4 with the following notation: \(n - k\), where the \(n\) represents the number of graph nodes and \(k\) denotes the number of colors.

A. Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm, introduced originally in Ref. [11], is considered to be one of the most promising approaches towards using near-term quantum computers for practical application. Its experimental feasibility has been recently demonstrated by a current Google experiment [31].

The purpose of QAOA is to find an approximate solution ground-state energy of a classical cost Hamiltonian \(H_c\), which usually encodes some combinatorial problem. The algorithm starts with applying Hadamard gates on all qubits, i.e., the state of the system is initially transformed to \(|+\rangle^\otimes N\).

Next, we apply sequentially the cost Hamiltonian \(H_c\) and a mixer Hamiltonian \(H_m\) for time-parameters \(\beta_i\) and \(\gamma_i\), respectively. After \(p\) iterations, the resulting state is of the
Machine learning framework [50] combined with TensorFlow. We found that in deep QAOA circuits the backpropagation method provided by TensorFlow showed a better convergence rate than the Parameter-shift rule, while in shallow circuits both methods have the same performance.

B. Comparison of Standard and Space-Efficient QAOA

Let us now compare the results for a coloring problem first solved by i) a standard QAOA approach presented in Sec. II-B and then by ii) a space-efficient QAOA with the method presented in Sec. III. The considered problem is the 3-coloring of Graph A, shown in Fig. 4a.

Looking at the convergence characteristics, the first problem was solved with a level-10 QAOA algorithm, using a circuit of 12 qubits, resulting in a circuit depth of 170. The convergence shown in Fig. 4 is towards the zero energy level, as we the shifted minimum energy eigenvalue to this value. For the coloring problem, when the gap reaches a size less than 0.75, the corresponding solution gives a correct coloring of the graph with probability 0.25. For the original algorithm, this energy level is reached at iteration no. 240, while the enhanced algorithm of space-efficient QAOA reaches the same level already at iteration no. 44 - showing a substantial improvement in the performance. Another metric to characterize the performance gain of the new algorithm is the overall CPU time usage. In this metric, the enhancement is showing an improvement of increasing execution speed by 75 times. Moreover, the new method decreased the memory usage by a factor of 3.47.

Taking the probability distribution over the best circuit solution, we can calculate the probability of measuring a state corresponding to a good coloring solution. We find the probabilities to be 0.557 for the original circuit, and 0.883 for our space-efficient algorithm.

The depth of a single QAOA level for the enhanced circuit is 37, whereas for the original circuit this number is 17. However, the enhanced algorithm needs only a level-6 QAOA, using a circuit of 8 qubits. Hence, although the total depth is increased, this enlargement is not that substantial and the number of required qubits and the needed iterations is far less.

C. Application of Stochastic Gradient Descent

We also studied the convergence properties of both the gradient descent with exact Hamiltonian expectation values and the stochastic gradient descent (SGD) [51], [52] obtained from estimating the expectation value from only a finite number of shots. For this investigation, we considered the coloring problem of Graph B represented in Fig. 4b with $k = 4$ colors. During the simulations, we used a level-6 QAOA, which has a circuit depth of 354. We found that after the optimization, the probability of measuring a bitstring representing a good coloring of Graph B is 0.845.

As shown in Fig. 5 the convergence of the true gradient descent optimization approaches the global minimum value with an energy distance of 0.75 already at the iteration no. 13, while the SGD with 50 and 100 shots at iterations 10
and 17, respectively. The global minimum is approached with a distance of 0.5 after 32 iterations when using the true gradient descent method and at iteration steps 11 and 43 by using SGD with 50 and 150 number of shots, respectively. That is, the SGD performed on par with the gradient descent using exact expectation values, and it would require only 150 measurements per iterations much less than one.

D. Evaluation of the 6-node, 4-color problem on Graph C

Here we present our findings on the evaluation problem of Graph C, which is the coloring task described in Fig. 4c. In this more complex example, we looked for the successful coloring (with \( k = 4 \) colors) of the 6-node graph. To simulate this problem using the space-efficient embedding technique, it is enough to consider a circuit containing only 12 qubits. A fast convergence can be achieved by only using a level-9 QAOA algorithm which is, once again, lower than the requirements for the simplest problem Graph A solved with the standard embedding. While the convergence pattern is different from the ones seen in Fig. 4a and Fig. 7, we observe significant improvement in convergence characteristics. The QAOA output energy reaches the theoretical minima within 0.1 gap in only 100 iterations. Our simulations show that the observed probability of finding the correct solution is as high as 97.4\%. These results represent a performance improvement of 97.3\% as compared to the Graph A simulation in Sec. V-B in terms of CPU time required.

VI. CONCLUSION AND OUTLOOK

We introduced a space-efficient embedding for quantum circuits solving the graph coloring problem. Through a series of investigations, we presented the performance gain of this method. We showed the limitations of the existing QA hardware solutions and then with various numerical simulations compared the standard and enhanced QAOA circuits. The required circuit width to embed the coloring problem is exponentially reduced in the number of colors; and although the depth of a single QAOA layer is increased, the number of required layers and optimization iteration steps to reach optimal solution are also decreased. The presented method and comparative study can be extended to a benchmarking framework for such performance gain analyses. Furthermore, analogous space-efficient embedding techniques could be used to improve upon other graph-related quantum optimization methods. We leave this for future work.

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