On The Variational Perspectives To The Graph Isomorphism Problem

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This paper studies the Graph Isomorphism Problem from a variational algorithmic perspective, specifically studying the Quadratic Unconstrained Binary Optimization (QUBO) formulation of the Graph Isomorphism Problem and subsequent execution using the Quantum Approximate Optimization Algorithm (QAOA) and the Variational Quantum Eigensolver (VQE). This study presents the results of these algorithms and the variations that occur therein for graphs of four and five nodes. The main findings of this paper include the clustering in the energy landscape for the QAOA in isomorphic graphs having an equal number of nodes and edges. This trend found in the QAOA study was further reinforced by studying the ground state energy reduction using VQEs. Furthermore, this paper examines the trend under which isomorphic pairs of graphs vary in the ground state energies, with varying edges and nodes.

1. INTRODUCTION

Hybrid quantum classical algorithms have emerged as a leading strategy to obtain quantum advantage in Noisy Intermediate Scale Quantum (NISQ) devices (Preskill 2018). One can mention variational quantum algorithms (VQAs), where the cost function is evaluated in the quantum circuit whose parameters are optimized by classical methods. The main advantage of VQAs is that they provide a general framework for a class of problems (Cerezo et al. 2021) (Lucas 2014). Typically in VQA the goal is to find a quantum state, which minimizes the energy of a problem Hamiltonian. Variational Quantum Eigensolver (VQE) (Peruzzo et al. 2014), and Quantum Approximate Optimization Algorithm (QAOA) (Farhi et al. 2014) are among the most remarkable examples of VQAs.

Meanwhile, quantum annealing (QA) provides us with an alternate way to enable quantum-enhanced information processing with the same areal application as VQAs. The key difference between VQAs and QA is that the former is a gate-based computation, and the latter is quantum-fluctuation-based computation exploiting quantum mechanical effects such as tunneling and entanglement. Quantum Annealers are relatively easier to build and have significantly more qubits than gate-based quantum devices. Physical qubits in Quantum Annealers are also not equivalent to the ones in gate-based quantum devices (Venegas-Andraca et al. 2018).

The concept of Quantum Annealing is based on the adiabatic theorem in physics, which involves slowly evolving the ground state of a physical system from the problem Hamiltonian of the system. Quantum annealing is the underlying principle for finding the ground state energy of a QUBO Problem. In Quantum Annealers, the problem Hamiltonian is represented as a Quadratic Unconstrained Binary Optimization (QUBO) problem (San...
Studying existing literature, it has been found that different QUBO formulations for the Graph Isomorphism Problem have been provided by Lucas (Lucas, 2014), Kenneth (Zick et al., 2015), Calude (Calude et al., 2017) etc. Kenneth and Calude performed their GI QUBO formulation experiments on D-Wave’s Quantum Annealer machines. It has been conjectured that the lowest number of logical qubits required for the general Graph Isomorphism Problem for two graphs of order n is $n^2$. Apart from GI using QUBO a class of Problems such as Boolean satisfiability (Farhi et al., 2000), binary clustering (Bauckhage et al., 2017), classifier training (Pudenz and Lidar, 2013), Travelling Salesman Problem (Salehi et al., 2021), vehicle routing (Borowski et al., 2020), railway dispatching problem (Domino et al., 2021) is been solved. Inspired by the results from the works mentioned earlier, this paper’s authors decided to try out the Graph Isomorphism Problem using QAOA and VQE.

This work presents the first study of the Graph Isomorphism Problem in the circuit model of quantum computation, according to the best of the authors’ knowledge of scientific literature in the field. The aims of this paper include:

1. Studying the variational formulations for the Graph Isomorphism Problem and its consequent implementation using the QAOA and the VQE.
2. Studying energy landscapes of the QAOA and the VQE.

2. BACKGROUND

For this paper, we try out two existing quantum approach to the Graph Isomorphism Problem: QAOA and VQE. QUBO formulation was used to get the problem Hamiltonian for QAOA and VQE. The motivation behind using these methods for the Graph Isomorphism Problem is described in the following subsections.

2.1. The Graph Isomorphism Problem

The Graph Isomorphism Problem is the computational problem of determining whether two finite graphs are structurally identical or isomorphic. An isomorphism of a graph $G = (V, E)$ to a graph $H = (W, F)$ is a one-to-one, bijective mapping from the vertex set of the first graph to the vertex set of the second graph.
FIG. 2: The illustration of variation in QAOA energies with simultaneous edge and node reduction. (a) Shows how edges were methodically removed from a five node complete graph (the graphs are reduced from (j) → (a)). A copy of each graph was used when testing, thereby yielding a pair of identical graphs, on which the graph isomorphism formulation was carried out. (b) Shows the QAOA energies of the Hamiltonian for each of these graphs for which the isomorphic pairs has the quadratic program yield a function value of zero.

V to the vertex set of the second graph W that preserves adjacency and non-adjacency. It is one of the very few unsolved Problems in NP. The exact complexity of the problem has eluded researchers ever since its conception for more than five decades. The problem is not known to be solvable in polynomial time or NP-complete. It may be put in the classical complexity class NP-complete. Interestingly, for many special classes of graphs, the problem can be solved in polynomial time. If the graphs have different sizes or orders, then they cannot be isomorphic, and these cases can be decided quickly. The current best known classical algorithm for the problem has a time complexity of \( \exp \left( (\log n)^{O(1)} \right) \) which is quasipolynomial. (Babai 2016) The quantum computational complexity of the problem is still unknown. (Shehab and au2 2017)

Previous attempts using quantum algorithms in the light of Hidden Subgroup Problem, using Quantum Fourier Sampling has been proven to fail. (Hallgren et al. 2010) (Grigni et al. 2001) (Shehab and au2 2017)

The Graph Isomorphism Problem has numerous applications in a variety of fields including the study of chemical compound structure, computational biology, where a graph representing a molecular compound must be compared to an entire database, social network security and many more.

2.1.1. The Quantum Approximate Optimization Algorithm

QAOA introduced by Farhi et al. (Farhi et al. 2014) finds an approximation to the ground state of a problem Hamiltonian by constructing a specific variational ansatz through first order Suzuki-Trotter decomposition approximating adiabatic evolution. The operators \( \exp(-i\beta H_m) \) and \( \exp(-i\alpha H_o) \) are applied in alternation resulting in the state

\[
|\alpha, \beta\rangle = \prod_{k=1}^{L} \exp(-i\beta_k H_m)\exp(-i\alpha_k H_o)|+\rangle \otimes^n,
\]

where \( H_o \) is the objective and \( H_m = -\sum_j X_j \) is the mixer Hamiltonian. Under fixed number of layers (i.e. \( L \)), the algorithm requires \( 2L \) parameters. The expectation value \( \langle \alpha, \beta | H | \alpha, \beta \rangle \), of state \( |\alpha, \beta\rangle \) is approximated through measuring the state in the computational basis. The parameters \( \alpha, \beta \) are updated using classical optimization procedure so that the energy is returns optimal value.

On one hand, QAOA can be utilized to solve a class of Problems such as Max-Cut (Farhi et al. 2001) (Majumdar et al. 2021), Max-k-Vertex Cover (Cook et al. 2020), at the same time, the applicability of QAOA extends to integer factorization problem (Anschuetz et al. 2018).
2.1.2. The Variational Quantum Eigensolver

The VQE uses Ritz’s variational principle to prepare the ground state and the corresponding energy. In this algorithm, the quantum computer is used to prepare variational trial states \( |\psi(\theta)\rangle = U(\theta)|0\rangle \), that depend on a set of parameters \( \theta \). Then, the expectation value of the energy \( \langle \psi(\theta)|H|\psi(\theta)\rangle \), is estimated and used by a classical optimization procedure to generate a new set of parameters. The advantage of VQE over classical simulation methods is that we can efficiently prepare trial states that are not tractable classically. VQE has a class of applications in physics (Mohtashin et al. 2021), chemistry, optimization Problems, and many more.

3. FORMULATION OF QUADRATIC PROGRAM

The first described baseline penalty Hamiltonian for the graph isomorphism was introduced in Lucas (Lucas 2014). Let us consider \( G_1 = (V_1, E_1) \), and \( G_2 = (V_2, E_2) \) graphs, where \( V \) are the vertices and \( E \) edges. The Hamiltonian is formulated by proposing binary variables \( x_{u,i} \), which is 1 if the vertex \( v \) in \( G_2 \) gets mapped to vertex \( i \) in \( G_1 \) as follows.

\[
H = A \sum_v \left( 1 - \sum_i x_{v,i} \right)^2 + A \sum_i \left( 1 - \sum_v x_{v,i} \right)^2 + B \sum_{ij \notin E_1 \cup E_2} x_{u,i} x_{v,j} + B \sum_{ij \in E_1 \cup E_2} x_{u,i} x_{v,j}.
\]  

In Zick et al. (Shehab and an2 2017) a modified formulation of Eq.2 is proposed in order to achieve a simple set of coupler values (e.g. 0, 1 instead of 0, 1, 2 in Lucas et al. 2017) amenable to quantum annealing. An edge related penalty is applied to a coupling iff there is not a vertex mapping penalty. The modified Hamiltonian is given as follows.

\[
H = A \sum_v \left( 1 - \sum_i x_{v,i} \right)^2 + A \sum_i \left( 1 - \sum_v x_{v,i} \right)^2 + B \sum_{ij \notin E_1 \cup E_2} x_{u,i} x_{v,j} + B \sum_{ij \in E_1 \cup E_2} x_{u,i} x_{v,j}.
\]

In Calude (Calude et al. 2017) a different methods for constructing efficient QUBO formulations for the Graph Isomorphism Problem. The objective for the formulation is given as follows.

\[
F(x) = H(x) + \sum_{ij \in E_1} P_{i,j}(x),
\]  

where

\[
H(x) = \sum_{0 \leq i < n} \left( 1 - \sum_{0 \leq i' < n} x_{i,i'} \right)^2 + \sum_{0 \leq i' < n} \left( 1 - \sum_{0 \leq i < n} x_{i,i'} \right)^2
\]

and

\[
\sum_{ij \in E_1} P_{i,j}(x) = \sum_{0 \leq i' < n} \sum_{0 \leq j' < n} x_{i,j'} (1 - e_{i',j'}),
\]  

e_{i,j} = 1 if \( ij \in E_2 \) and \( e_{i,j} = 0 \) if \( ij \notin E_2 \). This direct formulation of the quadratic function is done such that a mapping \( f \) can be decoded from that values of the variables in the quadratic program using a partial function

\[
D, \text{ such that } D : \mathbb{Z}_2^n \rightarrow \mathcal{F}, \text{ where } \mathcal{F} \text{ is the set of all bijections between } V_1 \text{ and } V_2. \text{ The domain of } D \text{ consists of all vectors } x \in \mathbb{Z}_2^n. \text{ Calude et. al. ensures that the function } H(x) = 0 \text{ if and only if } D \text{ is defined (and bijective). The component } \sum_{ij \in E_1} P_{i,j}(x) = 0 \text{ if and only if the mapping } f = D(x) \text{ is edge invariant. Therefore the function } F(x) = 0, \text{ for all } x \in \mathbb{Z}_2^n \text{ if and only if } f = D(x) \text{ is an isomorphism.}
\]

4. METHODOLOGY

The methodology for each experiment is different but was done on a common dataset unless stated otherwise. The data generator uses the NetworkX library and generates pairs of isomorphic and non-isomorphic connected graphs. For graphs having four nodes, the edge count remains in between four and five. On the other hand, for graphs having five nodes, all the graphs have five edges. Since the size of the QUBO matrix for a connected pair of graphs having \( N \) nodes is \( N \times N \), thereby utilizing \( N^2 \) qubits, the problem size was kept small for the NISQ era.
FIG. 3: The illustration of the energy for VQE (y-axis) for pairs of graphs with four nodes in respect with number of iterations (x-axis). The colors represent different runs on a class of graphs. It can be seen that after 400 iterations the energies cluster.

hardware simulations and computational constraints.

The QUBO matrix was generated using GSGMorph [11] and Technologies, [2021] from which the quadratic programs were obtained. For each set of problem instances, the offset value for all experiments is determined empirically such that the problem yields an optimal function value of 0 when the graphs are isomorphic, and the optimal function would raise a positive value when the graphs are non-isomorphic.

4.1. Numerical Setup for QAOA

The QAOA was implemented in Qiskit using the QAOA class and utilized the quadratic program formulated by Calude et al. [Calude et al., 2017]. The quadratic program was parsed in IBM’s Docplex model, which was used to feed it into the QAOA class. The QAOA utilized a minimum eigensolver interface that computed a minimum eigenvalue for the Hamiltonian thus generated by the quadratic program, with the number of layers in the QAOA being unity.

4.2. Numerical Setup for VQE

The Variational Quantum Eigensolver utilizes the VQE class in Qiskit. The quadratic program was parsed in IBM’s Docplex model, which was used to feed it into the VQE class. The VQE utilizes the TwoLocal ansatz consisting of RY and CZ gates with five repetitions and linear entanglement. The SPSA optimizer was used with a maximum iteration of 600 subjected to MinimumEigenOptimizer class.

5. RESULTS AND DISCUSSION

5.1. QAOA Results

The energies calculated are of the minimum eigenvalues of the converted problem Hamiltonian from the initial quadratic Docplex model using the MinimumEigenOptimizer class that takes the quadratic model and converts them into a tensor product of Pauli matrices. The corresponding minimum energy eigenvalues of the Hamiltonian for which the quadratic program yields a minimum eigenvalue of zero are given in Figure 1(a). Similarly, for graphs with five nodes, the energies are presented in Figure 1(b).

Extending on the results by Szegedy [Szegedy, 2019], in the light of the Ising formulation of the Graph Isomorphism Problem, solved using the QAOA, we observe that the energies for graphs having the same node count have roughly the same energies, as is evident from the graphs. Moreover, the number of edges have roughly the
same energies, with the energies values being distributed in a space having a relatively small value of standard deviations. Furthermore, Szegedy’s result [Szegedy 2019] states that for a MAX-CUT formulation of the QAOA, two isomorphic graphs will yield the same energy values given the same parameters for the QAOA quantum circuit. These results attempt to generalize that approach by showing that families of isomorphic graphs have energies within a very short deviation range. We will attempt to formalize this argument in the future iterations of this work.

However, in an experiment conducted as part of this study that takes two identical complete graphs and attempts to methodically remove one edge at random without replacement, varying the number of edges and the number of nodes in the graph simultaneously yields the results given in figure 2 (b). It is observed that as the number of edges and nodes is decreased, the energy values decrease till edge number 6, but weirdly energy increases from that point as the number of nodes and edges are reduced.

5.2. VQE Results

The results of the QAOA were supported by the results of the VQE, which yielded an optimal function value of zero for isomorphic graphs and non-zero for non-isomorphic pairs. It is noted that by using Variational Quantum Eigensolver, the ground state energies are not only much less(with absolute energy values being much greater than the QAOA), but the inherent trend of the energies found by either method is reflected herein. In other words, VQE results also corroborate the study that families of isomorphic graphs have energies within a very short deviation range. However, the optimization results from the VQE are obtained at a much higher time and resource cost.

6. CONCLUSION AND FUTURE WORK

As a summary, we have tested two different quantum algorithms QAOA and VQE, for the Graph Isomorphism Problem, where Hamiltonian is established using the QUBO formulation. We have shown through numerical simulations that the results of both algorithms support each other in identifying isomorphic and non-isomorphic pairs for four, and five nodes in a non-noisy device. Thus, we have proposed a new application area for these two quantum algorithms.

We have shown a few empirical pieces of evidence that agree with previous literature [Szegedy 2019] that QAOA energies of isomorphic graphs cluster together. Additionally, we have also shown that similar phenomena happen for VQE simulations as well. As per our knowledge, this phenomenon was not explored in the case of VQE before this work.

A further investigation of this work can be conducted by expanding the idea of energies clustering for families of isomorphic graphs and running the formulation on real devices.

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