Design of quantum approximate optimization algorithm for graph multi coloring problem

Gunsik Min
School of Electrical Engineering
Korea University
Seoul, Korea
lmgs3351@korea.ac.kr

Jun Heo
School of Electrical Engineering
Korea University
Seoul, Korea
junheo@korea.ac.kr

***Abstract*—We propose a technique to solve the problem of graph multi coloring, which is a problem corresponding to channel allocation problem, with the quantum approximate optimization algorithm(QAOA). QAOA is an algorithm that solve an optimization problem. Among the optimization problems, this algorithm is specialized as solving the quadratic unconstrained binary optimization(QUBO) problems. It is designed to find approximate solutions to combinatorial optimization problems by leveraging quantum resources. In general, it is evaluated to have strengths in optimizing the base of optimal path exploration, small factor resolution, and mass data exploration. The study on coloring problem using digital algorithm has solved the problem of coloring by replacing the graph with simple graph or applying algorithm or reducing the number of nodes. Despite these efforts, however, the digital algorithm that solves the coloring problem studied so far has not achieved satisfactory performance by some limitations. Therefore, in order to overcome these limitations, this paper will show the result of solving multi coloring problem by reducing initial state dimension of the QAOA**

I. INTRODUCTION

Quantum Approximate Optimization Algorithm(QAOA) is a quantum algorithm designed to solve the combinatorial optimization problems using near-term Noisy Intermediate Scale Quantum(NISQ) devices[1]. One of the challenging problems in this algorithm is the coloring problem, also known as graph coloring problem[2]. Graph coloring problem involves assigning colors to the vertices of given graph (G, E). The way is that no two adjacent vertices are assigned same color[3-5]. The goal is to assign all colors to the vertices of graph while adhering to the adjacency constraint. In this paper we propose the scheme for solving multi coloring problem which assigns the multi colors to the each vertices by QAOA. We also propose a quantum circuit method that reduces the QAOA level by making the corresponding input data.

II. PREVIOUS WORKS

In this section, we introduce the QAOA and multi coloring problem.

A. QAOA(Quantum Approximate Optimization Algorithm)

In defining the problem in terms of classical problem, we use N bit binary vector $\boldsymbol{z} = (z_1, \dots, z_N) \in \{\pm 1\}^N$binary vector x_i which is a vector for maximizing the classical objective function and define following function. Furthermore, we define the following cost function as H_C, which transforms it into Hamiltonian.

QAOA is designed by substituting the value obtained through the α −objective function of the above equation into the approximate ratio to maximize. Based on this method, quantum algorithm encode the problems by converting objective functions into quantum Hamiltonian.

$$C(\boldsymbol{z}) = \sum_{\alpha} C_{\alpha}(\boldsymbol{z}) \tag{1}$$

We first prepare the input data of the algorithm using the Hadamard quantum operator to create $|+\rangle^{\otimes n}$. This input data corresponds to the mixing Hamiltonian, H_M also called mixer.

$$H_M = \sum_{i} \sigma_i^x \tag{2}$$

The operator σ_i^x corresponds to the Pauli-X operator applied to the qubit associated with vertex i. Then the cost function corresponds to the problem Hamiltonian, H_C. Once the problem Hamiltonian is defined,

$$H_C = \sum_{i,j} \frac{w_{ij}}{2} \left(I - \sigma_i^z \sigma_j^z\right) \tag{3}$$

The quantum operator σ_i^z represents the Pauli-Z operator applied to the qubit corresponding to vertex i.

Based on these two types of Hamiltonians, the algorithm proceeds through a computational process to design the wavefunction as follows :

$$|\psi(\gamma,\beta)\rangle = e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} \dots e^{-i\beta_p H_M} e^{-i\gamma_p H_C} |\psi_0\rangle \quad (4)$$

The values γ, β are variables obtained through parameter optimization on a classical computer. Using the designed wavefunction, the expectation value for H_C is obtained, and the obtained approximation from the executed algorithm is compared. This iterative process involves repeatedly performing, refining the values of γ and β, and comparing with the approximation ratio achieved through the algorithms' execution.

$$F(\gamma,\beta) = \langle\psi(\gamma,\beta)|H_C|\psi(\gamma,\beta)\rangle \quad (5)$$

$F(\gamma,\beta)$ is the expected value of the quantum state obtained after applying quantum operations. This value is computed by substituting into the cost function using a classical computer. Finally, QAOA unfolds by designing optimized variables (γ,β) on a classical computer. Through wavefunction calculations, these variables yield optimized expected values, thus completing the optimization process.

B. Multi coloring problem

Graph coloring problem can be broadly divided into multi-coloring and single-coloring problems. In the context of graph theory, multi-coloring refers to situations where nodes in a graph can be colored with more than one color, while single-coloring implies that nodes can only be colored with one specific color.

Given k coloring graph $G(V,E)$, we define

$$\phi : V \to \{1,\dots,k\} \quad (6)$$

that assign different values to adjacent vertices

$$\{u,v\} \in E \to \phi(u) \neq \phi(v) \quad (7)$$

III. PROPOSED METHOD

Given graph $G(V,E)$, first we assume that the set of available total colors for coloring is denoted as $K \in \{1,\dots,k\}$ and the set of vertices is denoted as $V \in \{1,\dots,n\}$. Similarly, each node is replicated according to the size of coloring set. Each vertex set is assigned to $V = \{V_1, V_2, \dots, V_n\}$ and colorable set of each vertex to $\phi_{V_1}^K = \{\phi_{V_1}^1, \phi_{V_1}^2, \dots, \phi_{V_1}^k\}$.

$$\{i,j\} \in E \to \phi_{V_i}^K \neq \phi_{V_j}^K \quad (8)$$

As shown in above, i,j is adjacent vertex index. This means every copies of each vertex have to satisfy the above conditions. We will mention later about this condition in cost function Hamiltonian.

Then, the total number of qubits we have to assign is kn that we have to prepare the number of qubits. Let's consider an example of the input states. When the n-th node is assigned 2 colors out of the total 3 available colors, it is composed of two cases combined together. The first case involves adding a new color to the scenario where only 1 color out of the total 2 colors is assigned. The second case involves adding a new color and not assigning it in the situation where 2 colors out of the total 2 colors are already assigned. Therefore, the following superimposed states are generated:

$$|\psi_{n,3,2}\rangle = \sqrt{\frac{2}{3}}|\psi_{n,2,1}\rangle|1\rangle + \sqrt{\frac{1}{3}}|\psi_{n,2,2}\rangle|0\rangle$$
$$= \sqrt{\tfrac{2}{3}} \cdot \sqrt{\tfrac{1}{2}}(|01\rangle + |10\rangle) \otimes |1\rangle + \sqrt{\tfrac{1}{3}}(|11\rangle) \otimes |0\rangle \quad (9)$$

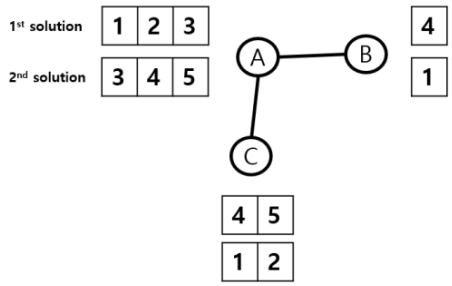

Fig. 1 Example of three vertices multi coloring problem

Before applying the algorithm, we prepare the input state as W-state. When the total number of colors available for coloring in a given graph is k, and the n-th node

$$|\psi_{n,k,l}\rangle = |\psi_{k,l_1}\rangle \otimes |\psi_{k,l_2}\rangle \otimes \dots \otimes |\psi_{k,l_n}\rangle \quad (10)$$

can be colored with l different colors. $|\psi_{k,l_1}\rangle$ is the state where denotes l of k colorable n-th vertex state. The input vector states can be prepared by superposition state $|\psi_{n,k,l}\rangle$

$$|\psi_{n,k,l}\rangle = \frac{1}{\sqrt{C_{k,l}}}(|1\dots10\dots0\rangle + \dots + |0\dots01\dots1\rangle) \quad (11)$$

In the given conditions, a total of state are superposition with equal probability.

$$C_{k,l} = \binom{k}{l} \quad (12)$$

These states are composed of k qubits, and among them, l qubits are assigned value of 1. This means each quantum states has hamming weight of l.

The choice of input state can affect the form of the mixing Hamiltonian used in the algorithm. In our case, we have chosen to apply XY mixer. XY mixer is expressed as follows :

$$H_{XY} = \frac{1}{2}\sum_{i,j\in T} \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \quad (13)$$

H_{XY} is mixing Hamiltonian which is consists of σ^x and σ^y pairs. The set T represents the mixing set, which includes all the coloring pairs for each vertex.
The operator σ_i^y in the above Hamiltonian is Pauli-Y operator.

$$\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y = |10\rangle\langle 01|_{ij} \tag{14}$$

If the state before applying above operator is $|00\rangle$ or $|11\rangle$, it is removed from the computational space. In other words, states within the infeasible space, such as the following states, are removed. Therefore, W-state can be applied as the input state as shown in Fig. 2.

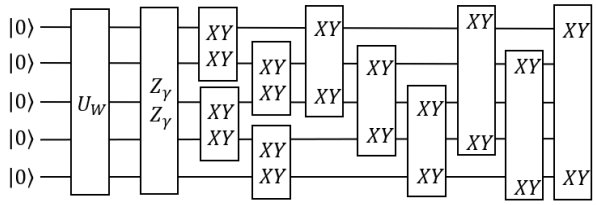

Fig. 2 QAOA applied $\boldsymbol{XY}$ mixer. Following $\boldsymbol{U_W}$ is $\boldsymbol{W}$ −state input preparation, $\boldsymbol{Z_\gamma Z_\gamma}$ represents problem Hamiltonian operator, and $\boldsymbol{XY}$ corresponds to $\boldsymbol{XY}$ mixing Hamiltonian.

The cost function Hamiltonian of QAOA solving graph coloring addresses the edge constraints. Let H_P be the problem Hamiltonian addressing edge constraints and Q_{ij} be the given graph G matrix.

$$H_P = \sum_K \sum_{(i,j)\in E} Q_{ij}\left(I - \sigma^z_{\phi^K_{V_i}} \sigma^z_{\phi^K_{V_j}}\right) \tag{15}$$

This means every copies of vertex have to satisfy the edge constraints.
For solving

$$\max_{\phi_V^K} C(\phi_V^K) = \sum_\alpha C_\alpha(\phi_V^K) \tag{16}$$

we define $C(\phi_V^K)$ as max multi colorable problem cost function corresponding to the problem Hamiltonian.
The desired state of level-p QAOA is expressed in the following state :

$$|\psi(\gamma,\beta)\rangle = e^{-i\beta_1 H_{XY}} e^{-i\gamma_1 H_P} \dots e^{-i\beta_p H_{XY}} e^{-i\gamma_p H_P} \tag{17}$$

Finally, expectation value is calculated as :

$$F(\gamma,\beta) = \langle\psi(\gamma,\beta)|H_P|\psi(\gamma,\beta)\rangle \tag{18}$$

The variable γ and β are determined through classical optimization, and ultimately, an iterative algorithm is performed in a direction that maximizes the approximation ratio, R

$$R = \frac{F(\gamma,\beta)}{F_{max}} \tag{19}$$

It is expected that lower levels of QAOA would exhibit higher performance. However, the complexity of adopting the proposed state as an input states need to be assessed. This is because conventional QAOA constructs the input state using single qubit operators. On the other hand, the proposed approach involves a significant number of Toffoli gates and two qubit unitary gates, which contribute to a substantial portion of the circuit depth. Therefore, it's important to examine the complexity introduced by the process of using the proposed state as an input data.

IV. Conclusion

In this paper, the fundamental concepts of QAOA were explained. Furthermore, a design approach for the input state dimensional reduction quantum algorithm process is proposed to solve the graph coloring problem. QAOA capable of addressing multi-coloring problems was discussed. By applying the quantum algorithm to multi-node allocation problems, it is expected to achieve high performance with a reduced number of iterations. However, for actual verification, simulations based on the proposed design need to be conducted to compare performances. Additionally, further research is required to understand at what QAOA level the performance saturates in the future.

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