Proper Cost Hamiltonian Design for Combinatorial Optimization Problems: A Boolean Function Approach

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***Abstract*—Advanced researches on the variational quantum algorithms are actively conducted. In particular, the quantum approximate optimization algorithm (QAOA) is one of the promising variational quantum algorithms and can be applied to various graph-based problems, and is a promising algorithm that shows good performance even in small quantum computers. As is widely known, QAOA obtains the approximate solution via the expectation value of the cost Hamiltonian on the parameterized state. Therefore, in addition to finding the optimal parameters, the proper design of the cost Hamiltonian is important. This paper designs the cost function of the combinatorial optimization problem via Boolean function and maps it to the proper cost Hamiltonian. The proposed cost Hamiltonian design method is applied to the maximum independent set (MIS) and minimum dominating set (MDS) problems.**

***Index Terms*—QAOA, MIS, MDS**

I. Introduction

One of the hottest quantum computing topics of the noisy intermediate-scale quantum (NISQ) era is the variational quantum algorithm [1]–[5]. Since the variational quantum algorithm uses a small number of qubits and resources, it has the advantage that it can exhibit good performance even in a small-scale quantum computer, so various researches are being conducted [6]. The quantum approximate optimization algorithm (QAOA) is one of the representative variational quantum algorithms along with variational quantum eigensolver (VQE) [7]–[9]. QAOA is a well-known promising hybrid quantum-classical optimizer, working as follows:

1) Design the cost Hamiltonian H_C of the problem based on the cost function $F(x)$.
2) Prepare the mixing Hamiltonian H_M composed of the Pauli-X matrix to be applied for each qubit.
3) Construct the parameterized state $|\gamma, \beta\rangle$ from the initial state $|s\rangle$ as follows:
$$|\gamma, \beta\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |s\rangle . \tag{1}$$
4) Obtain the solution samples via measurements of the expectation value of H_C on $|\gamma, \beta\rangle$ as follows:
$$\langle F(x)\rangle_{\gamma,\beta} = \langle \gamma, \beta | H_C | \gamma, \beta\rangle . \tag{2}$$
5) Search and update the parameters in the classical optimization loop until finding the optimal solution.

Note that, in Equation (1), p represents the depth of the QAOA circuit, and in the shallow circuit, the performance gets better as p increases [7], [10].

In the QAOA process, the proper design of the cost Hamiltonian is very important. Thus, this paper proposes a proper cost Hamiltonian design method using the Boolean Hamiltonian. In the first step, the cost function including objective and constraint for the combinatorial optimization problem is designed using the proper Boolean function. Then, the cost Hamiltonian is designed by mapping the Boolean function in the cost function to the Boolean Hamiltonian. The proposed design method is very intuitive and simple and can be applied to various problems.

The remainder of this paper is organized as follows. Section II describes the details of the cost Hamiltonian design method for the maximum independent set (MIS) problem. Section III describes the details of the cost Hamiltonian design method for the minimum dominating set (MDS) problem. Section IV concludes the paper.

II. Cost Hamiltonian for the Maximum Independent Set Problem

In this section, the cost function of the MIS problem is designed via Boolean functions. The designed cost function is mapped to the cost Hamiltonian using the relationship of the Boolean function and Boolean Hamiltonian. In particular, Boolean AND Hamiltonian is used for representing the constraint.

A. Cost Function Design

Consider an undirected graph $G(V, E)$ where V is a set of vertices and E is a set of edges. Here, $V = \{x_1, x_2, \cdots, x_n\}$, $x_m \in \{0, 1\}$, and $1 \leq m \leq n$. The goal is to maximize the independent set $V_I \subseteq V$ such that every vertex in V_I is not

TABLE I: Relationship of the Boolean function and Boolean Hamiltonian. $-$, $\wedge$, $\vee$, I, and Z represent the Boolean NOT, AND, OR, identity matrix, and Pauli-Z matrix, respectively. Details of the Boolean Hamiltonian derivation process can be found in [11], [12].

$\boldsymbol{f(x)}$	$\boldsymbol{H_f}$
x	$\frac{1}{2}(I-Z)$
$\overline{x}$	$\frac{1}{2}(I+Z)$
$x_1 \wedge x_2$	$\frac{1}{4}(I-Z_1-Z_2+Z_1Z_2)$
$\wedge_{j=1}^{n} x_j$	$\prod_{j=1}^{n}\frac{1}{2}(I-Z_j)$
$x_1 \vee x_2$	$\frac{1}{4}(3I-Z_1-Z_2-Z_1Z_2)$
$\vee_{j=1}^{n} x_j$	$I-\prod_{j=1}^{n}\frac{1}{2}(I+Z_j)$
$\overline{x}_1 \wedge \overline{x}_2$	$\frac{1}{4}(I+Z_1+Z_2+Z_1Z_2)$
$\wedge_{j=1}^{n} \overline{x}_j$	$\prod_{j=1}^{n}\frac{1}{2}(I+Z_j)$

adjacent to each other. Therefore, the cost function C_1 for the MIS problem can be designed as follows:

$$\begin{aligned} \max:\ C_1 &= \sum_{\forall (j,k)\in E}\left(\frac{x_j}{d_j}+\frac{x_k}{d_k}-2\delta(x_j \wedge x_k)\right) \\ &= \sum_{\forall x_j \in V} x_j - \delta^* \sum_{\forall (j,k)\in E}(x_j \wedge x_k), \quad (3) \end{aligned}$$

$$\text{where}\quad x_j = \begin{cases} 1, & \text{if } x_j \text{ is in } V_I, \\ 0, & \text{otherwise.} \end{cases} \quad (4)$$

Here, $j \in \mathbb{Z}^+$, $k \in \mathbb{Z}^+$, x_j is the jth vertex, d_j is the vertex degree of x_j, $\delta \geq 1$ is a large positive number, and $\wedge$ is a Boolean AND operator. In C_1, which should be maximized, the first term $\sum_{\forall x_j \in V} x_j$ and second term $-\delta^* \sum_{\forall (j,k)\in E}(x_j \wedge x_k)$ represent the objective term and the constraint term, respectively. At one edge, by Boolean AND function, the constraint term has a value of $-\delta^*$ only when both x_j and x_k are 1, and 0 otherwise. In other words, if both end vertices of one edge are in V_I, the cost is decreased by δ^*. This is a large minus-penalty to avoid the prohibition condition of MIS. The objective term increases the cost by the number of vertices included in V_I. Therefore, in (3), the constraint term induces V_I to become an independent set, and the objective term induces V_I to have more vertices.

B. Cost Hamiltonian Design

The cost Hamiltonian can be created by mapping the Boolean function part of the cost function to the Boolean Hamiltonian. According to TABLE I, the cost function C_1 is mapped to the following cost Hamiltonian H_{C_1} and should be maximized:

$$\begin{aligned} H_{C_1} &= \sum_{\forall x_j \in V}\frac{1}{2}(I-Z_j) \\ &\quad -\delta^* \sum_{\forall (j,k)\in E}\frac{1}{4}(I-Z_j-Z_k+Z_jZ_k), \quad (5) \end{aligned}$$

where I represents the identity matrix and Z_j represents the Pauli-Z matrix applying on the jth vertex (qubit) [13].

The extended version of H_{C_1} for the maximum weight independent set (MWIS) problem can be designed by replacing x_j with $w_j x_j$. More details of the simulation result of QAOA using the cost Hamiltonian of the MWIS problem can be found in [12], [14].

III. Cost Hamiltonian for the Minimum Dominating Set Problem

In this section, the cost Hamiltonian of the MDS problem is designed via Boolean Hamiltonian. In particular, Boolean NOR Hamiltonian is used for representing the constraint.

A. Cost Function Design

Consider an undirected graph $G(V,E)$ where V is a set of vertices and E is a set of edges. Here, $V=\{x_1,x_2,\cdots,x_n\}$, $x_m \in \{0,1\}$, and $1 \leq m \leq n$. The goal is to minimize the dominating set $V_D \subseteq V$ such that every vertex not in V_D is adjacent to at least one member of V_D. Therefore, the cost function C_2 for the MDS problem can be designed as follows:

$$\begin{aligned} \min:\ C_2 &= \sum_{\forall x_j \in V}\left\{\left(\sum_{\forall x_k \in A(j)}\frac{x_k}{1+d_k}\right)\right. \\ &\qquad \left. +\rho \wedge_{\forall x_k \in A(j)} \overline{x}_k\right\} \\ &= \sum_{\forall x_j \in V} x_j + \rho \sum_{\forall x_j \in V} \wedge_{\forall x_k \in A(j)} \overline{x}_k, \quad (6) \\ \text{where } A(j) &= \{x_j \text{ and all vertices adjacent to } x_j\}, \quad (7) \\ x_j &= \begin{cases} 1, & \text{if } x_j \text{ is in } V_D, \\ 0, & \text{otherwise.} \end{cases} \quad (8) \end{aligned}$$

Here, $j \in \mathbb{Z}^+$, $k \in \mathbb{Z}^+$, x_j is the jth vertex, $A(j) \subseteq V$, d_k is the vertex degree of x_k, $\rho \geq 1$ is a large positive number, $\wedge$ is a Boolean AND operator, and $-$ is a Boolean NOT operator. In C_2, which should be minimized, the first term $\sum_{\forall x_j \in V} x_j$ and second term $\rho \sum_{\forall x_j \in V} \wedge_{\forall x_k \in A(j)} \overline{x}_k$ represent the objective term and the constraint term, respectively. In particular, the constraint term of C_2 is designed as the Boolean NOR operation of itself and all adjacent vertices. Thus, at one vertex, the constraint term has a value of ρ only when both its and adjacent vertices are all 0, and 0 otherwise. In other words, if at least one vertex among itself and adjacent vertices are not included in V_D, the cost is increased by ρ. This is a large plus-penalty to avoid the prohibition condition of MDS. The objective term counts the number of vertices included in V_D. Therefore, in (6), the constraint term induces V_D to become a dominating set, and the objective term induces V_D to have fewer vertices.

B. Cost Hamiltonian Design

According to TABLE I, the cost function C_2 is mapped to the following cost Hamiltonian H_{C_2} and should be minimized:

$$H_{C_2} = \sum_{\forall x_j \in V} \frac{1}{2}(I - Z_j) + \rho \sum_{\forall x_j \in V} \left(\prod_{\forall x_k \in A(j)} \frac{1}{2}(I + Z_k) \right), \quad (9)$$

where I represents the identity matrix and Z_j represents the Pauli-Z matrix applying on the jth vertex (qubit) [13].

C. Experimental Results

In order to solve the MDS problem, the experiments were performed by applying H_{C_2} to QAOA at the shallow circuit depth $p = 1, 3, 5, 7, 9$. A set of 8-vertex 3-regular graphs and a set of 10-vertex 3-regular graphs were generated with 10 instances each. 1000 measurements were taken for each instance. The experiments were performed using TensorFlow Quantum and Cirq [15]. Adam optimizer was used to optimize the parameters of QAOA [16].

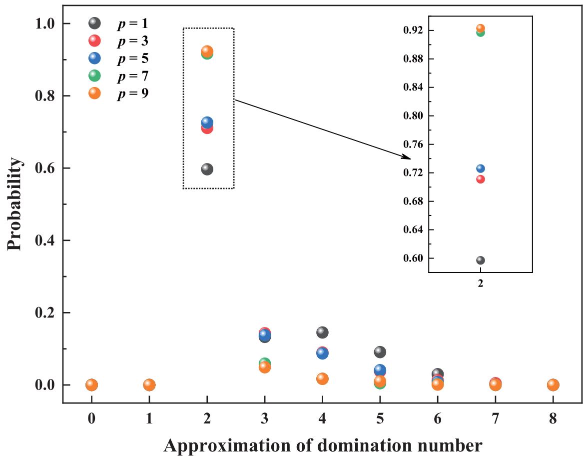
Fig. 1a shows the approximate solution (the approximation of domination number) of the MDS problem for 10 instances of the 8-vertex 3-regular graph set and the average probability that each solution was obtained. The optimal solution (the real domination number) of all 10 instances of the 8-vertex 3-regular graph set obtained via brute-force search was 2. The optimal solution 2 was obtained the most in all p.

Fig. 1b shows the approximate solution of the MDS problem for 10 instances of the 10-vertex 3-regular graph set and the average probability that each solution was obtained. The optimal solution of all 10 instances of the 10-vertex 3-regular graph set obtained via brute-force search was 3. The optimal solution 3 was obtained the most in all p.

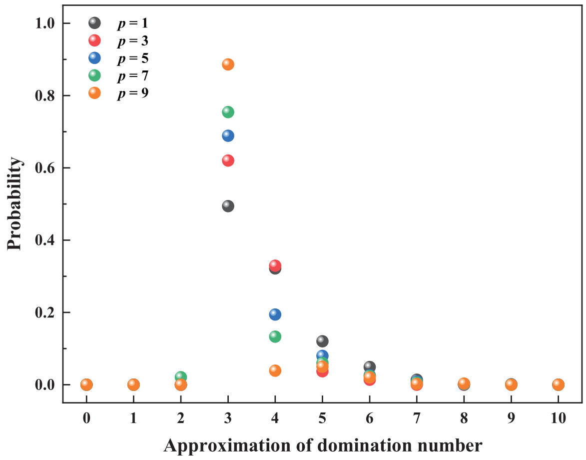
Fig. 2 shows the optimal solution ratio according to p. In both the 8-vertex and 10-vertex 3-regular graphs, as p increases, the optimal solution ratio increases. At $p = 1$, the optimal solution ratio of the 8-vertex and 10-vertex 3-regular graphs are about 60% and 50%, respectively. And at $p = 9$, the optimal solution ratio of both graphs reaches about 90%. Therefore, it was confirmed via experimental results that the design of the cost Hamiltonian H_{C_2} for the MDS problem was proper.

IV. Conclusion

This paper proposed a cost Hamiltonian design method using the Boolean function. The cost functions for the MIS and MDS problems were designed using Boolean functions. Based on the cost functions, cost Hamiltonians for the MIS and MDS problems were designed using the relationship between a Boolean function and a Boolean Hamiltonian. In particular, it was confirmed that the cost Hamiltonian for the MDS problem was applied to QAOA to show good performance. The proposed cost Hamiltonian design method will be useful for various combinatorial optimization problems.



(a)



(b)

Fig. 1: (a) Average probability of approximation of domination number on 8-vertex 3-regular graphs according to circuit depth p. The real domination numbers of 10 instances obtained via brute-force search are all 2. (b) Average probability of approximation of domination number on 10-vertex 3-regular graphs according to circuit depth p. The real domination numbers of 10 instances obtained via brute-force search are all 3.

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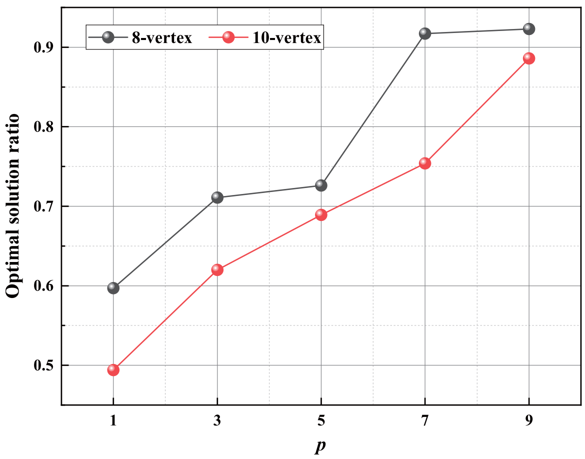

Fig. 2: Average optimal solution ratio of 8-vertex and 10-vertex 3-regular graphs. As the circuit depth p increases, the optimal solution ratio tends to increase.

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