

Application of Quantum Approximate Optimization Algorithm in Solving the Total Domination Problem

Haoqian Pan ^{a,1,*}, Shiyue Wang^a, Changhong Lu^a

^a*School of Mathematical Sciences, Key Laboratory of MEA (Ministry of Education) &
Shanghai Key Laboratory of PMMP, East China Normal
University, Shanghai, 200241, China*

Abstract

Recent advancements in quantum computing have led to significant research into applying quantum algorithms to combinatorial optimization problems. Among these challenges, the Total Domination Problem (TDP) is particularly noteworthy, representing a classic and critical example in the field. Since the last century, research efforts have focused on establishing its NP-completeness and developing algorithms for its resolution, which have been fundamental to combinatorial mathematics. Despite this rich history, the application of quantum algorithms to the TDP remains largely unexplored. In this study, we present a pioneering application of the Quantum Approximate Optimization Algorithm (QAOA) to tackle the TDP, evaluating its efficacy across a diverse array of parameters. Our experimental findings indicate that QAOA is effective in addressing the TDP; under most parameter combinations, it successfully computes the correct total dominating set (TDS). However, the algorithm's performance in identifying the optimal TDS is contingent upon the specific parameter choices, revealing a significant bias in the distribution of effective parameter points. This research contributes valuable insights into the potential of quantum algorithms for addressing the TDP and lays the groundwork for future investigations in this area.

Keywords:

Quantum approximate optimization algorithm, Total domination problem, Qiskit

*Corresponding author.

¹52215500040@stu.ecnu.edu.cn

1. Introduction

In recent years, advancements in quantum computing (Raussendorf and Briegel, 2001; Ladd et al., 2010; Fauseweh, 2024) have led to the development of various quantum algorithms, including the Quantum Approximate Optimization Algorithm (Farhi et al., 2014), the Quantum Adiabatic Algorithm (Albash and Lidar, 2018), and Quantum Annealing (Rajak et al., 2023). This progress has generated considerable interest in applying quantum algorithms to combinatorial optimization problems, such as the Max Clique Problem (Childs et al., 2000), Max Cut Problem (Farhi et al., 2014), Domination Problem (DP) (Guerrero, 2020), Max Flow Problem (Krauss et al., 2020), and Minimal Vertex Cover Problem (Zhang et al., 2022). Despite the growing enthusiasm for quantum algorithms in combinatorial optimization, there remains a notable gap in research on specific problems, particularly the Total Domination Problem (TDP). In graph theory, a dominating set (DS) for a graph $G(V, E)$ is defined as a subset $D \subseteq V$ such that every vertex $v \in V \setminus D$ has at least one neighbor in D . A total dominating set (TDS) further requires that no isolated vertices exist within D . The objective of the TDP is to identify the smallest such set D . Since the last century, significant strides have been made in studying TDP, with comprehensive reviews available in (Chang, 1998; Henning, 2009, 2013; Haynes et al., 2023). TDP has been established as NP-complete for various types of graphs, including general graphs, bipartite graphs, and comparability graphs (Pfaff et al., 1983), as well as split graphs (Laskar and Pfaff, 1983), chordal graphs (Laskar et al., 1984), circular graphs (Keil, 1993), line graphs, and line graphs of bipartite and claw-free graphs (McRae, 1994). Research into the NP-completeness of TDP has led to the development of algorithms tailored to specific graph classes, often aimed at minimizing time complexity. For instance, studies have investigated interval graphs (Breu and Kirkpatrick, 1996; Adhar and Peng, 1992), circular-arc graphs (Bertossi and Moretti, 1990; Rao and Rangan, 1989), cocomparability graphs (Breu and Kirkpatrick, 1996; Kratsch and Stewart, 1997), asteroidal triple-free graphs (Kratsch, 2000), distance hereditary graphs (Chang et al., 2002), and tree graphs (Henning, 2013). To date, however, the literature lacks investigations into the application of quantum computing techniques to the TDP. The potential of quantum algorithms to effectively solve TDP, as well as their performance metrics, remains an open question for future research.

In this context, this paper presents the first application of QAOA to solve TDP on a quantum simulator. We validated the effectiveness of QAOA

across 128 parameter combinations. The experimental results show that QAOA successfully computes the correct TDS for 93 of these combinations, with 12 combinations yielding the optimal TDS. Additionally, we found that under certain parameter settings, the accuracy of the final sampling results from QAOA can reach approximately 70%, while the optimal probability can approach 25%. Based on these results, we affirm that utilizing QAOA to solve TDP holds significant potential and merits further investigation. This work represents one of the earliest contributions to the application of quantum computing in addressing TDP, and our findings will provide valuable insights for subsequent research employing quantum algorithms for this problem.

The structure of this paper is as follows. In Section 2, we analyze TDP and present its 0-1 integer programming model, gradually deriving the process of converting it into a Hamiltonian. In Section 3, we outline the basic workflow of QAOA. Section 4 details our experiments using a quantum simulator on a 6-node graph, comparing the performance of QAOA in solving TDP across different parameter combinations. Finally, Section 5 provides a summary of the entire paper.

2. From TDP to Hamiltonian

This paper primarily investigates the use of QAOA to solve TDP. A key challenge in applying quantum algorithms to combinatorial optimization problems is effectively modeling these problems as Quadratic Unconstrained Binary Optimization (QUBO) models. The basic form of the QUBO model is presented in Eq. 1, where the matrix Q is referred to as the QUBO matrix.

$$\text{minimize/maximize } y = x^t Q x \quad (1)$$

In this chapter, we focus on presenting the QUBO formulation of the TDP problem. Our approach begins by modeling the TDP as a 0-1 integer programming problem. We convert the constraints of the 0-1 integer programming model into quadratic penalties and incorporate them into the original objective function, ultimately deriving the QUBO model. We start by providing a complete definition of the TDP problem. Given a graph $G(V, E)$, its TDS, denoted as D , is a subset of V that contains no isolated vertices. For every vertex $v \in V \setminus D$, there exists at least one vertex in D to which it is connected. The objective of the TDP is to find such a set D with the minimal size. Notably, unlike classical DP, TDP requires that there are no

isolated vertices within D . Next, we present the 0-1 integer programming model for the TDP.

$$\min_{\{X_i\}} \sum_{i=1}^{|V|} X_i \quad (2)$$

$$\text{s.t.} \quad \sum_{j \in N(i)} X_j \geq 1 \quad \forall i \in V \quad (3)$$

$$X_i \in \{0, 1\} \quad \forall i \in V \quad (4)$$

In this model, when a vertex $i \in D$, $X_i = 1$; otherwise, $X_i = 0$. The objective function in Eq. 2 represents the size of D . For each vertex i , it is important to note that the constraint in Eq. 3 utilizes the open neighborhood $N(i)$ instead of the closed neighborhood $N[i]$. In classical DP, the closed neighborhood would typically be used. However, for TDP, which requires that there are no isolated vertices in $G[D]$, each vertex in the dominating set D must have at least one neighbor that is also in D . This condition differentiates TDP from DP, making it more stringent.

With the 0-1 integer programming model for TDP established, we now proceed to convert this model into a QUBO formulation. Since $X_* \in \{0, 1\}$, it follows that $X_* = X_*^2$, which means the original objective function already meets the requirements of the QUBO model. Our next task is to convert the constraint in Eq. 3 into quadratic penalties and incorporate these penalties into the original objective function. The general form of Constraint 3 is as follows:

$$X_1 + X_2 + \cdots + X_n \geq 1, \quad n = |N(i)|, \quad \forall i \in V \quad (5)$$

When $n = 1$ or $n = 2$, we can transform them according to Glover et al. (2022) as follows:

$$P \cdot (X_1 - 1)^2 \quad \text{or} \quad P \cdot (1 - X_1 - X_2 + X_1 \cdot X_2)$$

Here, P is the punishment coefficient. When $n \geq 3$, we introduce a slack variable S to convert the inequality $X_1 + X_2 + \cdots + X_n \geq 1$ into an equality constraint.

$$X_1 + X_2 + \cdots + X_n - S - 1 = 0 \quad (6)$$

Since $X_1 + X_2 + \cdots + X_n - 1 \geq 0$ and $X_* \in \{0, 1\}$, it follows that $S \in [0, n-1]$, where S can take all integer values within this range. After estimating the

range of S , our next task is to represent S using additional 0-1 variables. Considering the range of S , we can express S as:

$$S = \sum_{i=1}^{bl_{n-1}-1} X'_i * 2^{i-1} + (n-1 - \sum_{i=1}^{bl_{n-1}-1} 2^{i-1}) * X'_{bl_{n-1}} \quad (7)$$

Here, the symbol bl_n denotes the length of the binary representation of the integer n . For example, $bl_3 = 2$ since the binary representation of 3 is 11. Additionally, $X'_* \in \{0, 1\}$ represents the newly introduced variables to express S . After completing these preparations, we can begin the conversion of Constraint 3 into quadratic penalties. First, we can rewrite Eq. 6 as follows:

$$P \cdot (X_1 + X_2 + \dots + X_n - S - 1)^2 \quad (8)$$

By substituting Eq. 7 into Eq. 8, we obtain:

$$P \cdot (X_1 + X_2 + \dots + X_n - [\sum_{i=1}^{bl_{n-1}-1} X'_i \cdot 2^{i-1} + (n-1 - \sum_{i=1}^{bl_{n-1}-1} 2^{i-1}) \cdot X'_{bl_{n-1}}] - 1)^2 \quad (9)$$

Finally, we arrive at the QUBO model for the TDP, which can be expressed as:

$$\begin{aligned} & \min_{\{X, X'\}} \sum_{i=1}^{|V|} X_i \\ & + \sum_{i \in V, |N(i)| \geq 3} P \cdot [\sum_{j \in N(i)} X_j - (\sum_{i=1}^{bl_{|N(i)|-1}-1} X'_i \cdot 2^{i-1} + (|N(i)| - 1 - \sum_{i=1}^{bl_{|N(i)|-1}-1} 2^{i-1}) \cdot X'_{bl_{|N(i)|-1}}) - 1]^2 \\ & + \sum_{i \in V, |N(i)|=2, N(i)=\{j,k\}} P \cdot (1 - X_j - X_k + X_j \cdot X_k) \\ & + \sum_{i \in V, |N(i)|=1, N(i)=\{j\}} P \cdot (X_j - 1)^2 \end{aligned} \quad (10)$$

At this point, we have completed the conversion of the TDP into a QUBO model. To utilize QAOA to solve this model, we need to convert it into a Hamiltonian. First, we need to convert all 0-1 variables X and X' into binary variables s that take values in $\{-1, 1\}$. The conversion is as follows:

$$X_i = \frac{s_i + 1}{2} \quad (11)$$

After the substitution, Eq. 10 becomes:

$$\begin{aligned}
& \min_{\{s, s'\}} \sum_{i=1}^{|V|} \frac{s_i + 1}{2} \\
& + \sum_{i \in V, |N(i)| \geq 3} P * \left[\sum_{j \in N(i)} \frac{s_j + 1}{2} \right. \\
& - \left(\sum_{i=1}^{bl_{|N(i)|-1}-1} \frac{s'_i + 1}{2} * 2^{i-1} + (|N(i)| - 1 - \sum_{i=1}^{bl_{|N(i)|-1}-1} 2^{i-1}) * \frac{s'_{bl_{|N(i)|-1}} + 1}{2} \right) - 1 \Big]^2 \\
& + \sum_{i \in V, |N(i)|=2, N(i)=\{j, k\}} P \cdot \left(1 - \frac{s_j + 1}{2} - \frac{s_k + 1}{2} + \frac{s_j + 1}{2} \cdot \frac{s_k + 1}{2} \right) \\
& + \sum_{i \in V, |N(i)|=1, N(i)=\{j\}} P \cdot \left(\frac{s_j + 1}{2} - 1 \right)^2
\end{aligned} \tag{12}$$

Next, by replacing s and s' with the **Pauli-Z operator σ^z** , we can ultimately obtain the Hamiltonian.

$$\begin{aligned}
H_c &= \sum_{i=1}^{|V|} \frac{\sigma_i^z + 1}{2} \\
& + \sum_{i \in V, |N(i)| \geq 3} P \cdot \left[\sum_{j \in N(i)} \frac{\sigma_j^z + 1}{2} \right. \\
& - \left(\sum_{i=1}^{bl_{|N(i)|-1}-1} \frac{(\sigma_i^z)' + 1}{2} \cdot 2^{i-1} + (|N(i)| - 1 - \sum_{i=1}^{bl_{|N(i)|-1}-1} 2^{i-1}) \cdot \frac{(\sigma_{bl_{|N(i)|-1}}^z)' + 1}{2} \right) - 1 \Big]^2 \\
& + \sum_{i \in V, |N(i)|=2, N(i)=\{j, k\}} P \cdot \left(1 - \frac{\sigma_j^z + 1}{2} - \frac{\sigma_k^z + 1}{2} + \frac{\sigma_j^z + 1}{2} \cdot \frac{\sigma_k^z + 1}{2} \right) \\
& + \sum_{i \in V, |N(i)|=1, N(i)=\{j\}} P \cdot \left(\frac{\sigma_j^z + 1}{2} - 1 \right)^2
\end{aligned} \tag{13}$$

At this point, we have completed the process of converting the TDP into a Hamiltonian, marking the completion of our preparations for using QAOA to solve the TDP. In the following chapters, we will introduce the basic concepts of QAOA.

3. QAOA

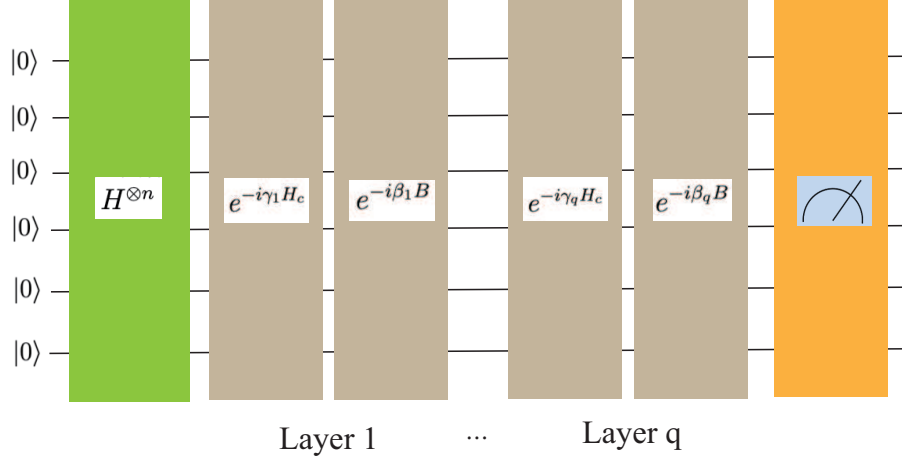


Figure 1: Working flow of QAOA.

We illustrate the basic concepts of the QAOA algorithm using Fig. 1. For a quantum system consisting of n qubits, we represent the state vector of this quantum system using the bit string z , where $z = z_1 z_2 z_3 \dots z_n$ and $z_i = 0, 1$, corresponding to the two different spin directions. The Hamiltonian of the system is H_c , which we derived from the QUBO model of TDP in the previous steps. This implies that we have mapped the objective function of a combinatorial optimization problem to the energy of a quantum system. The QAOA algorithm begins by using a Hadamard gate to prepare the initial state $|s\rangle$ from $\underbrace{|00\dots 0\rangle}_n$.

$$|s\rangle = \underbrace{\hat{H} \otimes \hat{H} \dots \otimes \hat{H}}_n \underbrace{|00\dots 0\rangle}_n = \frac{1}{\sqrt{2^n}} \cdot \sum_z |z\rangle \quad (14)$$

In the initial state $|s\rangle$, if we measure the wave function of the quantum system directly, the probability of the system collapsing into any state vector is $\frac{1}{\sqrt{2^n}}$. QAOA applies two types of unitary transformations, $U(C, \gamma)$ and $U(B, \beta)$ (Eq. 15, Eq. 16), to the initial state $|s\rangle$, repeating this process q times.

Here, $C = H_c$, $B = \sum_{j=1}^n \sigma_j^x$, $\gamma \in [0, 2\pi]$, and $\beta \in [0, \pi]$.

$$U(C, \gamma) = e^{-i\gamma H_c} \quad (15)$$

$$U(B, \beta) = e^{-i\beta B} \quad (16)$$

In Fig. 1, γ_q and β_q represent the two types of angles at the q -th layer. After repeating this process q times, we obtain the final state $|\gamma, \beta\rangle$.

$$|\gamma, \beta\rangle = U(B, \beta_q)U(C, \gamma_q) \cdots U(B, \beta_1)U(C, \gamma_1) |s\rangle \quad (17)$$

We can obtain the expected value of H_c , denoted as $F_q(\gamma, \beta)$, by repeatedly loading the circuit and measuring $|\gamma, \beta\rangle$ multiple times.

$$F_q(\gamma, \beta) = \langle \gamma, \beta | H_c | \gamma, \beta \rangle \quad (18)$$

Since the TDP is a minimization problem, we need to continuously adjust the angles γ and β at each layer to minimize $F_q(\gamma, \beta)$. QAOA is a hybrid algorithm that combines quantum computing with a classical optimizer, typically using classical optimizers such as COBYLA to adjust the angles at each layer. The optimization process concludes when the maximum number of iterations is reached or when a specified function tolerance is met. At this point, we obtain the optimal angles γ_* and β_* . We then use γ_* and β_* to update the quantum circuit and perform multiple samplings, outputting the bit string z_* with the highest probability from the sampling results. From z_* , we can extract the final TDS.

4. Experiment

The experimental environment utilizes an AMD R9 7950X3D CPU with 48 GB of memory. We employed IBM's Qiskit package to construct the QAOA quantum circuits, perform backend simulations, and conduct sampling. The optimizer used is COBYLA from the Scipy optimize package, with a default function tolerance of 10^{-8} . For the initial values of γ and β in QAOA, we adopted the initialization method proposed in Sack and Serbyn (2021). The graph used in this study is depicted in Fig. 2. This graph consists of six vertices, and the size of its minimal DS is 2, which can include $\{2,5\}$, $\{0,2\}$, $\{1,4\}$, or $\{4,0\}$. However, none of these sets meet the conditions for a TDS since all of them contain isolated vertices. Similar to minimal

DS, there are multiple minimal TDS, such as $\{0,1,2\}$, $\{0,4,5\}$, $\{1,2,4\}$, and $\{2,4,5\}$. Considering the different sizes of minimal DS and minimal TDS, this graph effectively helps us validate the performance of QAOA in solving the TDP rather than DP.

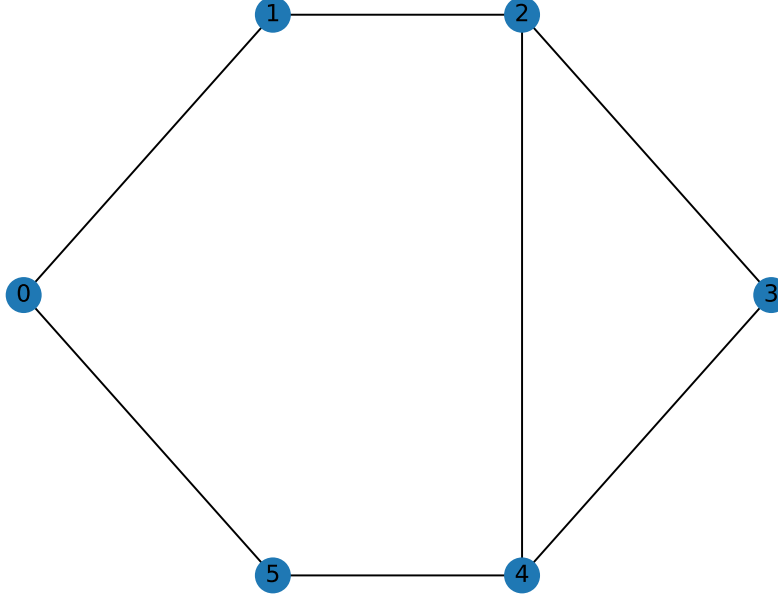


Figure 2: A graph with 6 nodes and 7 edges.

Additionally, based on the conversion method introduced in Section 2, the QUBO model for the TDP of this graph is given by Eq. 19. This model can be easily transformed into the Hamiltonian by substituting x_* with $\frac{s_*+1}{2}$ and replacing s_* with σ_*^z . For the sake of brevity, we will not expand on this here.

$$\begin{aligned}
\text{minimize} \quad & x_0 + x_1 + x_2 + x_3 + x_4 + x_5 \\
& + P \cdot (1 - x_1 - x_5 + x_1 \cdot x_5) \\
& + P \cdot (1 - x_0 - x_2 + x_0 \cdot x_2) \\
& + P \cdot (x_1 + x_3 + x_4 - (x_6 + x_7) - 1)^2 \\
& + P \cdot (1 - x_2 - x_4 + x_2 \cdot x_4) \\
& + P \cdot (x_2 + x_3 + x_5 - (x_8 + x_9) - 1)^2 \\
& + P \cdot (1 - x_0 - x_4 + x_0 \cdot x_4), \quad x_* \in \{0, 1\}
\end{aligned} \tag{19}$$

The parameters involved in the entire experiment include the layer number q , the punishment coefficient P , and the maximum iterations. To ensure the completeness of the testing, we evaluated the performance of QAOA in solving the TDP across a total of 128 parameter combinations, with $q \in \{2, 5, 10, 20\}$, $P \in \{4.8, 5.4, 6.6, 7.2, 7.8, 8.4, 9.0\}$, and maximum iterations $\in \{50, 100, 200, 500\}$. The values of P correspond to 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, and 1.5 times the total number of vertices. This choice of values is inspired by Glover et al. (2022).

First, we present some experimental results obtained under specific parameters. We set $q = 5$, $P = 9.0$, and maximum iterations = 500. Fig. 3 shows the probability distribution of bit strings from the final sampling results, with the bit string $z = 100011$ highlighted in purple due to its highest sampling probability of 0.0655. This bit string's sampling probability is noticeably higher than that of the others. By marking the corresponding vertex set $\{0, 4, 5\}$ in the graph (Fig. 4), we confirm that this bit string corresponds to a DS that meets the TDS conditions, and that this TDS is minimal. Additionally, in Fig. 3, we observe that the sampling probability for $z = 111000$ is 0.0653, making it the second highest probability bit string. Through visualization (Fig. 5), we see that the corresponding set $\{0, 1, 2\}$ forms another minimal TDS. Although our examination of the remaining bit strings in Fig. 3 did not reveal significantly higher probabilities for the two other potential TDS, $\{1, 2, 4\}$ and $\{2, 4, 5\}$, we can still affirm that QAOA is effective for solving the TDP under these parameters. In Fig. 6, we record the trend of cost variation throughout the iterations. We find that, between iterations $\in [0, 60]$, the cost fluctuates significantly. Once the number of iterations exceeds 60, the cost changes become more stable. This indicates that the QAOA exhibits good convergence when solving the TDP with the current parameters. We believe that the dramatic fluctuations in cost are due to the penalty terms in the Hamiltonian. Since the penalty must exceed the original objective function value, when COBYLA iterates through the angles, it faces situations where some penalty terms become zero while others back to non-zero. This causes sharp variations in cost. However, once most penalties are satisfied and reduced to zero, the cost changes become smoother. This transition signifies a shift in the optimization focus from finding a TDS to identifying a smaller TDS.

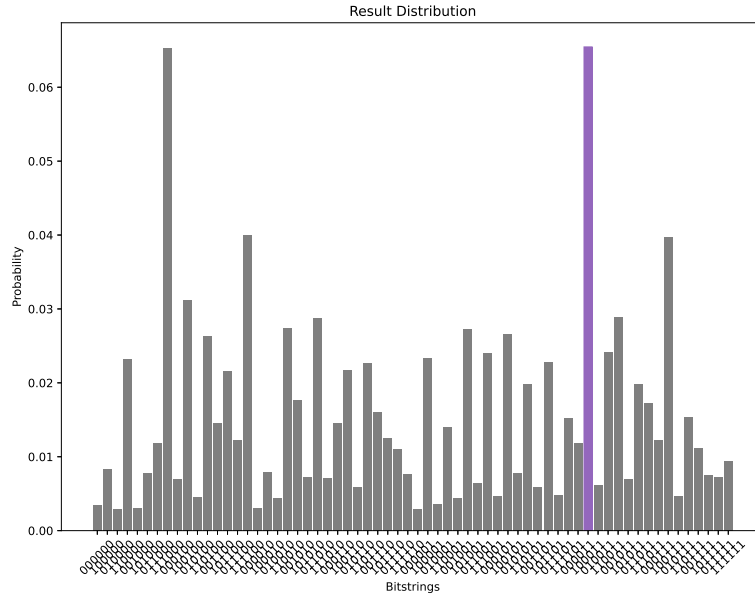


Figure 3: Probability distribution of the final sampling result when $q = 5$, $P = 9.0$, and maximal iterations = 500.

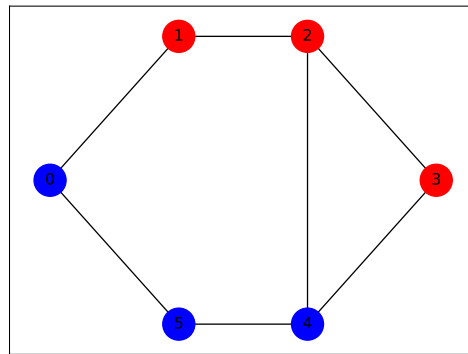


Figure 4: Visualization of the bit string 100011.

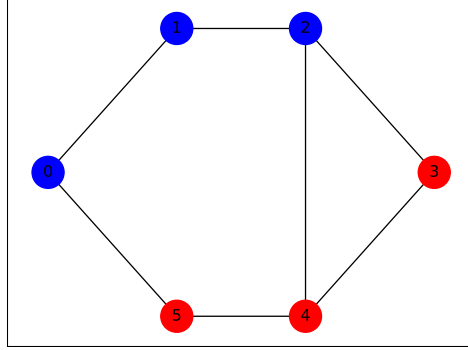


Figure 5: Visualization of the bit string 111000.

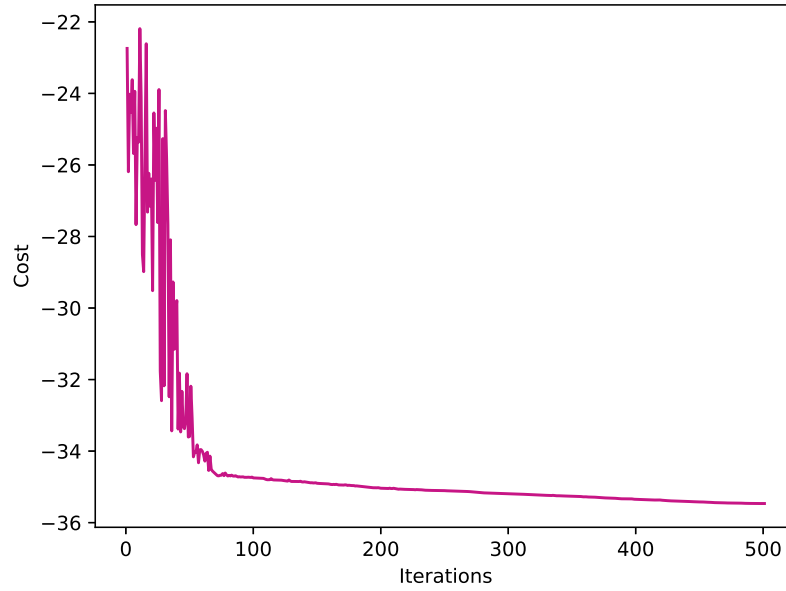


Figure 6: Cost of the QAOA when $q = 5$, $P = 9.0$, and maximal iterations = 500.

Next, we will present a comparison of QAOA computational results under different parameter configurations. First, in Fig. 7, we illustrate the

cost variations for different values of q . We observe that when the number of layers q is larger, such as $q = 10$ or 20 , the amplitude and range of cost fluctuations are greater compared to $q = 2$ and 5 . Even when the number of iterations reaches its maximum, the costs for $q = 10$ and 20 continue to fluctuate. We believe this is due to a significant number of penalty terms remaining non-zero after the initial fluctuations have ended. Additionally, the increased number of variables associated with more layers may lead the COBYLA algorithm to prematurely converge on local optima. We can confirm that, for the current instance we are using (Fig. 2), setting too many layers for QAOA is ineffective and may require more iterations. For $q = 2$ and $q = 5$, the cost clearly settles into a local optimum when $q = 2$. According to Farhi et al. (2014), we can derive Eq. 20, which indicates that as the number of layers q increases, the expected value of the sampled H_c approaches the size of the minimal TDS. We believe that in the current instance, the smaller values of q , such as 2 and 5, align with this trend. However, the number of layers, the chosen optimization algorithm, maximum iterations, punishment coefficient P , and other parameters may all limit the capabilities of the QAOA algorithm designed for larger layer structures. These bottlenecks could ultimately prevent the QAOA algorithm from finding better values for γ and β within the specified range of maximum iterations.

$$\lim_{q \rightarrow \infty} \min_{\gamma, \beta} F_q(\gamma, \beta) = \min |TDS| \quad (20)$$

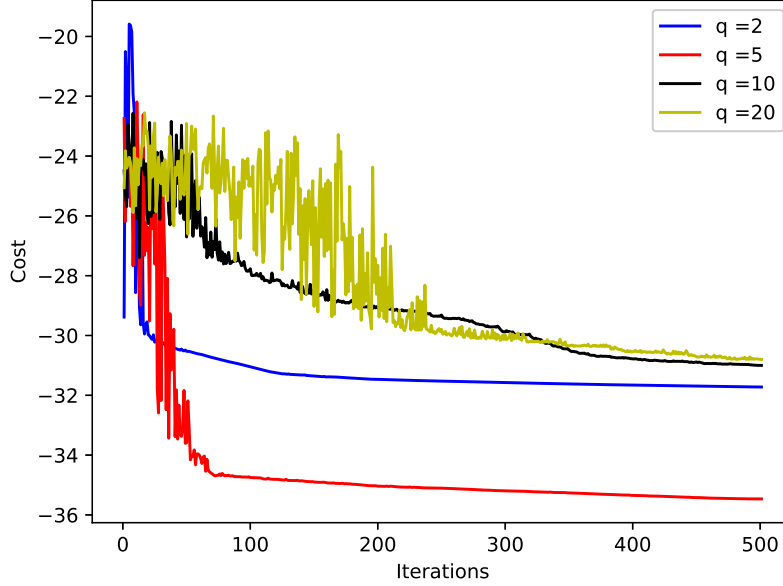


Figure 7: The comparison of cost for different q when $P = 9.0$ and maximal iterations = 500.

Next, in Figs. 8 and 9, we present the total probabilities of obtaining TDS (Correct probability) and minimal TDS (Optimal probability) from all sampled bit strings under different parameter combinations. Overall, we find that within the parameter ranges we set, the probability of QAOA successfully identifying TDS remains fairly stable, generally within the range of $[0.3, 0.7]$. Higher maximum iterations contribute to increasing the upper probability limit for finding TDS, leading us to conclude that the QAOA can relatively easily identify TDS. Regarding the optimal TDS, we observe that higher probabilities tend to cluster in regions with fewer layers, a trend that holds consistently across different levels of maximum iterations. Furthermore, among the parameter combinations yielding the highest probabilities, we notice that the punishment coefficients are generally larger. One possible explanation for this is that within a certain range, a larger punishment coefficient leads to more pronounced fluctuations in cost during the initial phases, which may assist classical optimization algorithms in escaping local optima during the optimization process.

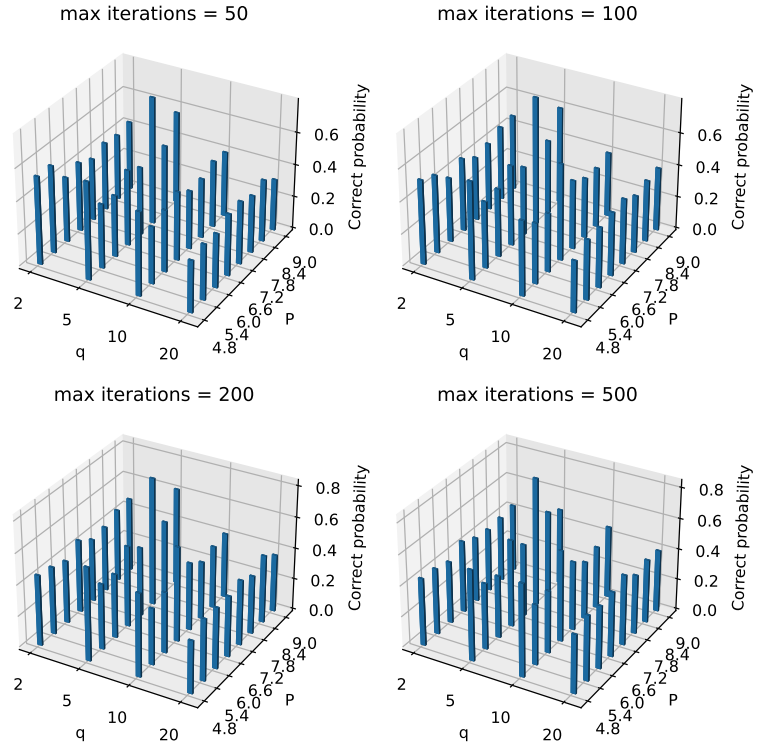


Figure 8: Correct probabilities for $q \in \{2, 5, 10, 20\}$, $P \in \{4.8, 5.4, 6.6, 6.6, 7.2, 7.8, 8.4, 9.0\}$ and maximal iterations $\in \{50, 100, 200, 500\}$.

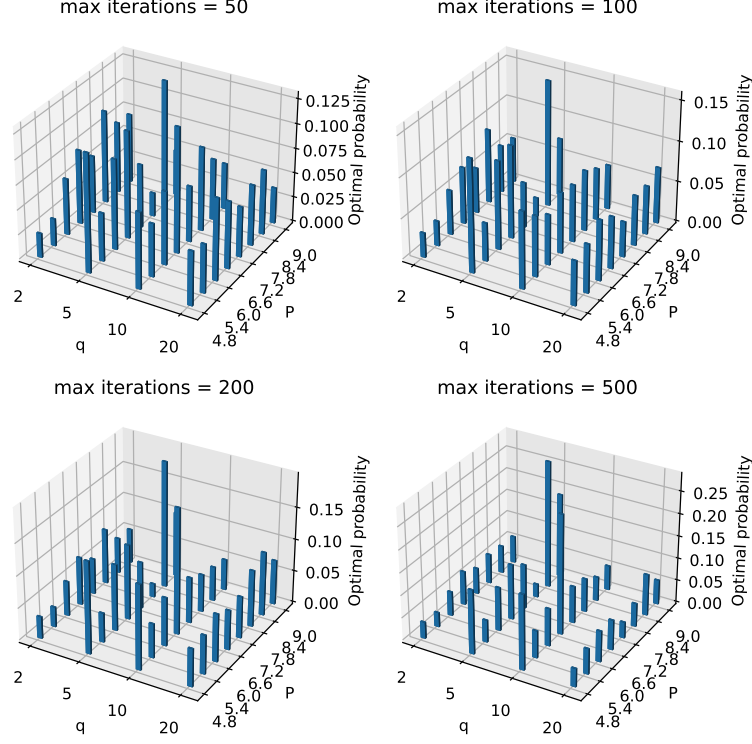


Figure 9: Optimal probabilities for $q \in \{2, 5, 10, 20\}$, $P \in \{4.8, 5.4, 6.6, 6.6, 7.2, 7.8, 8.4, 9.0\}$ and maximal iterations $\in \{50, 100, 200, 500\}$.

The results shown in Figs. 10 and 11 further validate this observation. In Fig. 10, we record the distribution of parameter points where z_* corresponds to TDS, while in Fig. 11, we document the distribution for minimal TDS. We find that out of 128 parameter combinations, 93 yielded TDS, with 12 resulting in minimal TDS. Additionally, the distribution of parameter points for TDS is quite uniform, whereas the distribution for minimal TDS exhibits a clear tendency, clustering in regions characterized by smaller q values and larger P values. This aligns with our earlier analysis. Based on these characteristics, we conclude that when using QAOA to solve TDP, it is quite efficient in finding a TDS and is relatively insensitive to parameter choices. However, to identify the optimal TDS, more careful selection of parameters

is necessary.

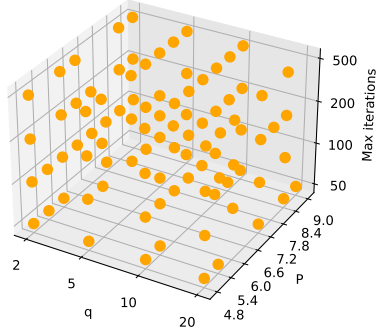


Figure 10: Parameter points for z_* which is a TDS.

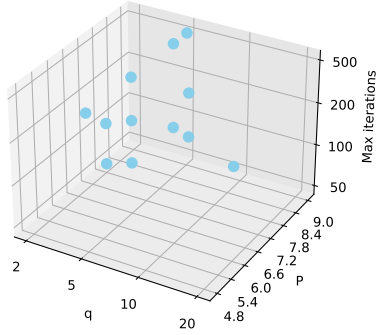


Figure 11: Parameter points for z_* which is a minimal TDS.

Additionally, in Table 1, we compare the time complexity of QAOA with other algorithms for solving TDP. Here, mis represents the maximal iterations of COBYLA, n denotes the number of vertices in the graph, and m refers to the number of edges. The time complexity analysis of QAOA has already been provided in Zhang et al. (2022). According to this analysis, the time complexity of QAOA consists of two components. The first component

is $O[\text{poly}(q)]$ (Zhou et al., 2020), which is related to the q -layer structure of the algorithm. The second component is associated with the time complexity of the classical optimization algorithm used. Since we employed COBYLA, its time complexity is $O[\text{poly}(mis)]$. Therefore, the overall time complexity is $O[\text{poly}(q) + \text{poly}(mis)]$. Comparing this with the algorithms listed in Table 1, we find that the time complexity of QAOA is acceptable. Although the algorithm may not currently have a clear advantage for specific classes of graphs, it is designed to be general-purpose, which provides an edge over other algorithms in terms of versatility. Moreover, this study did not optimize the quantum circuits, instead using those generated directly by IBM’s Qiskit. Additionally, we did not tailor or explore other classical optimization algorithms specific to the characteristics of the TDP. These factors indicate that there is significant potential for further development in this work.

Table 1: The comparison of time complexity of algorithms for TDP.

Algorithm	Time complexity	For specific graphs?
QAOA	$O[\text{poly}(q) + \text{poly}(mis)]$	no
Bertossi and Gori (1988)	$O(n \ln(n))$	interval graphs
Breu and Kirkpatrick (1996)	$O(nm^2)$	cocomparability graphs
Kratsch and Stewart (1997)	$O(nm^2)$	cocomparability graphs
Kratsch (2000)	$O(n^6)$	asteroidal triple-free graphs
Chang et al. (2002)	linear time	distance hereditary graphs
Henning (2013)	linear time	tree graphs

5. Conclusion

This paper investigates the use of QAOA to solve the TDP. We first model the TDP as a 0-1 integer programming problem, then convert the constraints into quadratic penalties and integrate them into the original objective function, resulting in the QUBO formulation for TDP. By further transforming the QUBO model into a Hamiltonian, we complete the preparation for solving the TDP using QAOA. We conducted detailed tests of QAOA’s performance on TDP using a quantum simulator across 128 parameter combinations. The results indicate that QAOA successfully computes correct TDS for most parameter settings, and in approximately 10% of cases, it outputs the optimal

TDS. This suggests that the ability of QAOA to find optimal TDS is dependent on the parameters used. Additionally, an analysis of the bit string probability distribution in the final sampling results under varying parameters reveals that the accuracy of QAOA remains relatively stable within our selected parameter range, while optimal probabilities tend to favor smaller layer numbers and larger punishment coefficients. Based on the current experimental findings, we conclude that using QAOA to solve TDP is feasible and has significant potential for further development, although a more detailed parameter analysis is necessary to enhance the likelihood of obtaining optimal TDS.

Based on the experimental results and analysis, we identify the limitations of this work as follows: (1) We did not optimize our quantum circuits according to the specific characteristics of the TDP; the circuits used were generated by IBM’s Qiskit. (2) The classical optimization algorithm employed could be further refined to minimize the required maximal iterations. (3) We did not conduct practical tests on a quantum computer.

Finally, we believe that the work presented in this paper can be extended in the following directions: (1) Conducting tests on quantum computers using QAOA or other quantum algorithms to evaluate the performance in a broader parameter range and across more test instances for solving the TDP. (2) Further enhancing the probability of QAOA successfully identifying the optimal TDS through detailed parameter range analysis, quantum circuit optimization, and exploring additional classical optimization algorithms. (3) Building on this work to apply the QAOA to solve other variants of the domination problem, such as perfect domination and k-domination.

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This work is inspired by the GitHub project named qopt-best-practices [<https://github.com/qiskit-community/qopt-best-practices.git>] while utilizing the QAOA. Additionally, all quantum programming tools employed in this study are derived from IBM’s Qiskit package.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of interest

The authors declare that they have no conflicts of interest that could have appeared to influence the work reported in this paper.

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Declaration of Generative AI

During the preparation of this work the authors used chatgpt in order to improve readability and language. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

References

- Adhar, G.S., Peng, S., 1992. Parallel algorithms for finding connected, independent and total domination in interval graphs, in: Proceedings of the international workshop on Algorithms and parallel VLSI architectures II, pp. 85–90.
- Albash, T., Lidar, D.A., 2018. Adiabatic quantum computation. Reviews of Modern Physics 90, 015002.
- Bertossi, A.A., Gori, A., 1988. Total domination and irredundance in weighted interval graphs. SIAM journal on discrete mathematics 1, 317–327.
- Bertossi, A.A., Moretti, S., 1990. Parallel algorithms on circular-arc graphs. Information Processing Letters 33, 275–281.
- Breu, H., Kirkpatrick, D., 1996. Algorithms for dominating and steiner set problems in cocomparability.
- Chang, G.J., 1998. Algorithmic aspects of domination in graphs. Handbook of Combinatorial Optimization: Volume1–3 , 1811–1877.

- Chang, M.S., Wu, S.C., Chang, G.J., Yeh, H.G., 2002. Domination in distance-hereditary graphs. WOS:000173568800006 URL: <https://ir.lib.nycu.edu.tw/handle/11536/29069>.
- Childs, A.M., Farhi, E., Goldstone, J., Gutmann, S., 2000. Finding cliques by quantum adiabatic evolution. arXiv preprint quant-ph/0012104 .
- Farhi, E., Goldstone, J., Gutmann, S., 2014. A quantum approximate optimization algorithm. URL: 10.48550/arXiv.1411.4028.
- Fauseweh, B., 2024. Quantum many-body simulations on digital quantum computers: State-of-the-art and future challenges. *Nature Communications* 15, 2123.
- Glover, F., Kochenberger, G., Hennig, R., Du, Y., 2022. Quantum bridge analytics i: a tutorial on formulating and using qubo models. *Annals of Operations Research* 314, 141–183.
- Guerrero, N.J., 2020. Solving combinatorial optimization problems using the quantum approximation optimization algorithm .
- Haynes, T.W., Hedetniemi, S.T., Henning, M.A., 2023. Domination in graphs: Core concepts. Springer.
- Henning, M., 2013. Total domination in graphs. Springer Monographs in Mathematics/Springer .
- Henning, M.A., 2009. A survey of selected recent results on total domination in graphs. *Discrete Mathematics* 309, 32–63.
- Keil, J.M., 1993. The complexity of domination problems in circle graphs. *Discrete Applied Mathematics* 42, 51–63.
- Kratsch, D., 2000. Domination and total domination on asteroidal triple-free graphs. *Discrete Applied Mathematics* 99, 111–123.
- Kratsch, D., Stewart, L., 1997. Total domination and transformation. *Information processing letters* 63, 167–170.
- Krauss, T., McCollum, J., Pendery, C., Litwin, S., Michaels, A.J., 2020. Solving the max-flow problem on a quantum annealing computer. *IEEE Transactions on Quantum Engineering* 1, 1–10.

- Ladd, T.D., Jelezko, F., Laflamme, R., Nakamura, Y., Monroe, C., O'Brien, J.L., 2010. Quantum computers. *nature* 464, 45–53. URL: <https://www.nature.com/articles/nature08812>.
- Laskar, R., Pfaff, J., Hedetniemi, S., Hedetniemi, S., 1984. On the algorithmic complexity of total domination. *SIAM Journal on Algebraic Discrete Methods* 5, 420–425.
- Laskar, R.C., Pfaff, J., 1983. Domination and irredundance in split graphs. Report.
- McRae, A.A., 1994. Generalizing NP-completeness proofs for bipartite graphs and chordal graphs. Clemson University.
- Pfaff, J., Laskar, R., Hedetniemi, S.T., 1983. NP-completeness of total and connected domination and irredundance for bipartite graphs. Clemson University Clemson, SC.
- Rajak, A., Suzuki, S., Dutta, A., Chakrabarti, B.K., 2023. Quantum annealing: An overview. *Philosophical Transactions of the Royal Society A* 381, 20210417.
- Rao, A.S., Rangan, C.P., 1989. Optimal parallel algorithms on circular-arc graphs, in: *International Conference on Foundations of Software Technology and Theoretical Computer Science*, Springer. pp. 44–55.
- Raussendorf, R., Briegel, H.J., 2001. A one-way quantum computer. *Physical review letters* 86, 5188. URL: <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.86.5188>.
- Sack, S.H., Serbyn, M., 2021. Quantum annealing initialization of the quantum approximate optimization algorithm. *quantum* 5, 491.
- Zhang, Y.J., Mu, X.D., Liu, X.W., Wang, X.Y., Zhang, X., Li, K., Wu, T.Y., Zhao, D., Dong, C., 2022. Applying the quantum approximate optimization algorithm to the minimum vertex cover problem. *Applied Soft Computing* 118. doi:10.1016/j.asoc.2022.108554.
- Zhou, L., Wang, S.T., Choi, S., Pichler, H., Lukin, M.D., 2020. Quantum approximate optimization algorithm: Performance, mechanism, and implementation on near-term devices. *Physical Review X* 10, 021067.