A variational quantum eigensolver (VQE) algorithm for optimal target selection in two-dimensional space

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ABSTRACT

This paper applies the variational quantum eigensolver (VQE) algorithm to solve the problem of optimal target selection in two-dimensional space. Specifically, we consider a system comprising multiple moving targets, each traveling in a straight line at a different constant speed and heading towards a fixed object A. The objective of the problem is to find the target with the minimum time of approach to the fixed object A. Although this problem can be solved efficiently by classical methods, the quantum method is proposed here to demonstrate the potential of quantum computing in solving more complex versions of combinatorial optimization problems. We focus on an in-depth analysis of encoding the classical problem into a quantum problem, constructing the objective function H (Hamiltonian), and detailing the procedural steps of the VQE algorithm.

Keywords: Quantum optimization; Target selection; Hybrid quantum-classical algorithm; NISQ.

1. INTRODUCTION

In many fields such as aviation surveillance, defense, and logistics, making optimal decisions based on real-time data is extremely important. One of the common problems is selecting the optimal target from a set of potential objects. Classical computing methods can effectively solve small-scale problems. However, as the number of targets increases, along with the complexity of constraints (e.g., targets capable of changing direction, noisy environments), the computational complexity of classical algorithms can increase exponentially, leading to infeasible solution times. With the advancement of quantum computing technology, quantum optimization algorithms such as VQE [1], QSE (Quantum Subspace Expansion) [2], and QAOA (Quantum Approximate Optimization Algorithm) [3] have opened new avenues for solving combinatorial optimization problems. Each algorithm has its own strengths and weaknesses, making it suitable for the varying requirements and complexities of specific problems. VQE is specifically designed to find the lowest eigenvalue of a Hamiltonian and is particularly well-suited for today's Noisy Intermediate-Scale Quantum (NISQ) computers, as it is a hybrid algorithm that combines classical and quantum processors [3, 4]. This approach helps to mitigate the impact of noise and errors on current quantum devices. This paper details the direct application of the VQE algorithm to solve for the optimal target defined by the shortest approach time. This study serves as a concrete methodology for how the variational quantum eigensolver can be structured to address real-world optimization challenges.

2. METHODOLOGY

2.1. Classical solution

To solve this problem using a classical method, we can use a simple algorithm with a linear complexity of O(N), where N is the number of targets. The steps are as follows:

- Initialization: Set a variable *min_time* to an infinite value and an *optimal_target* variable to store the index of the optimal target.

- Iteration: Iterate through each target T_i with i=1 to N.

- Time calculation: For each target T_i, calculate the approach time T_i based on its initial position and speed.

- Comparison and update: Compare the calculated time T_i with *min_time*. If it is smaller, update *min_time* to T_i and *optimal_target* to the current index i.

Result: After iterating through all targets, *optimal_target* will contain the index of the target with the minimum approach time.

The above solution is very effective and fast for simple problems; however, it does not take advantage of the ability to process and solve the problem in parallel.

2.2. Quantum method and parallel processing capability

In contrast to the classical method, quantum computing opens up the possibility of solving problems simultaneously and in parallel through the phenomenon of quantum superposition. When a quantum system is prepared in a superposition state, it can represent all potential solutions to the problem at the same time. For this problem, we can initialize a superposition state of all targets, representing the consideration of all targets simultaneously. Then, by applying quantum transformations (the VQE circuit), we can interact with this state in parallel to find the state with the lowest energy (corresponding to the minimum time). This mechanism allows the algorithm to explore the solution space much more efficiently than the sequential iteration of a classical computer, especially as the number of targets and the complexity of the problem increase.

2.3. Problem modeling

The problem is modeled in 2D space with the following components:

- Fixed object A: Position (x_A,y_A).

- Moving targets T_i (with i = 1, ..., N): Each target T_i has an initial position (x_{i0},y_{i0}) and moves in a straight line with a constant speed towards object A.

- Objective function: Minimize the time for the target T_i to move from the initial position (x_{i0} ,y_{i0}) to object A. This time is calculated by the formula:

$$T_i = \frac{d(T_{i0}, A)}{v_i} = \frac{\sqrt{(x_A - x_{i0})^2 + (y_A - y_{i0})^2}}{v_i} \tag{1}$$

The problem becomes finding the index i such that the time T_i is minimized.

2.4. Encoding the problem into a quantum model

To solve this problem with the VQE algorithm, we need to encode it into a Hamiltonian (H)

Quantum variables: We use N qubits to represent N targets. A qubit in the state $|1\rangle$ can represent the selection of the corresponding target, and $|0\rangle$ represents not selecting it. Because we only need to select a single target, the quantum state of the system will be a linear combination of the basis states $|0...1...0\rangle$ (with only one bit being 1).

Hamiltonian: The Hamiltonian of the system needs to reflect the objective function. The energy value of a basis state must correspond to the approach time of that target. We can construct the Hamiltonian (H) as a diagonal matrix, with the diagonal elements corresponding to the time T_i:

$$H = \sum_{i=1}^{N} T_i |i\rangle\langle i| \tag{2}$$

Where, $|i\rangle$ is the quantum state representing the selection of the i target. In the form of Pauli operators, we can represent this Hamiltonian using Pauli-Z operators. For N targets, corresponding to N qubits, the generalized Hamiltonian is written as follows:

$$H = \sum_{i=1}^{N} T_i \frac{I - Z_i}{2} = \left(\frac{1}{2}\sum_{i=1}^{N} T_I\right) I - \left(\frac{1}{2}\sum_{i=1}^{N} T_i Z_i\right) \tag{3}$$

The construction of this Hamiltonian requires a transformation from a combinatorial optimization problem (Ising model) to Pauli operators.

2.5. The VQE algorithm

The VQE algorithm is a hybrid algorithm that combines a classical and a quantum processor to find the smallest eigenvalue (ground state energy) of a Hamiltonian [3]. The two main components of VQE are the Ansatz circuit and the COBYLA (Constrained Optimization By Linear Approximation) optimizer.

Ansatz circuit: This circuit is designed to prepare a quantum state that approximates the ground state of the Hamiltonian. It consists of parameterized rotation gates Ry(θ) and CNOT gates. The CNOT gates generate entanglement between the qubits, allowing the algorithm to explore the solution space more effectively. Figure 1 shows a 3-layer Ansatz circuit.

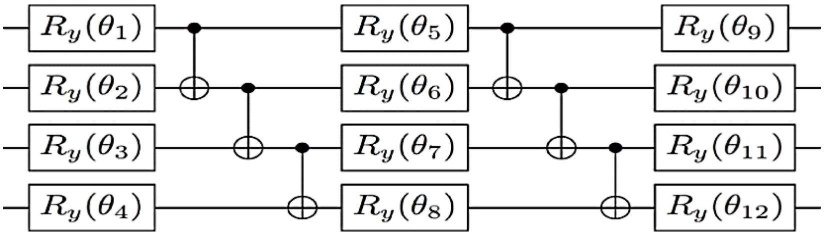

Figure 1. *3-layer Ansatz circuit [6].*

COBYLA optimizer: This is a derivative-free optimization algorithm that adjusts the parameters θ of the quantum circuit [5]. After receiving the energy value from the quantum computer, COBYLA uses this information to estimate an approximate linear model of the objective function. Based on this model, it finds a new set of parameters θ to continue reducing the energy value. The workflow of the COBYLA optimizer is illustrated in figure 2.

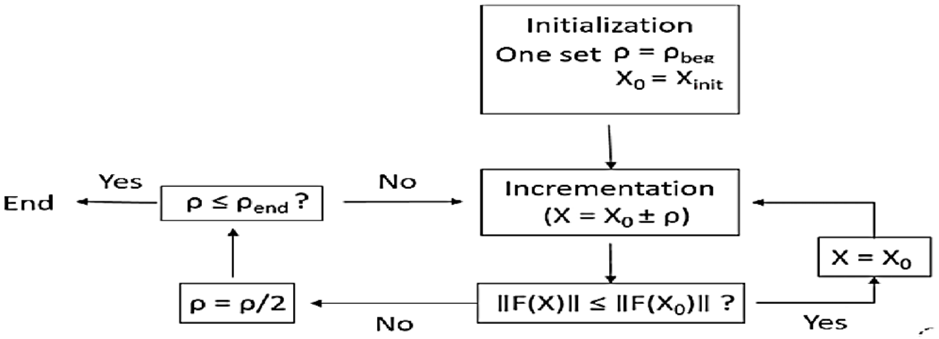

Figure 2. *COBYLA optimizer [5].*

The steps of the VQE algorithm are as follows:

- Ansatz circuit design: Construct a quantum circuit (Ansatz) U(θ) with adjustable parameters θ. This circuit is tasked with creating a quantum state close to the ground state of the Hamiltonian.

- Expectation value calculation: On the quantum computer, we prepare the initial state $|0\rangle$, then apply the circuit U(θ) to create the state $|\psi(\theta)\rangle = U(\theta)|0\rangle$. Next, we measure the expectation value of the Hamiltonian: $\langle H\rangle = \langle\psi(\theta)|H|\psi(\theta)\rangle$.

- Classical optimization: A classical optimizer (e.g., COBYLA, SLSQP) will be used to adjust the parameters θ of the Ansatz circuit to minimize the expectation value $\langle H\rangle$. This process is repeated until the minimum value of $\langle H\rangle$ is reached.

The smallest expectation value is the optimal approach time, and the corresponding parameters θ will give us the quantum state representing the optimal target choice.

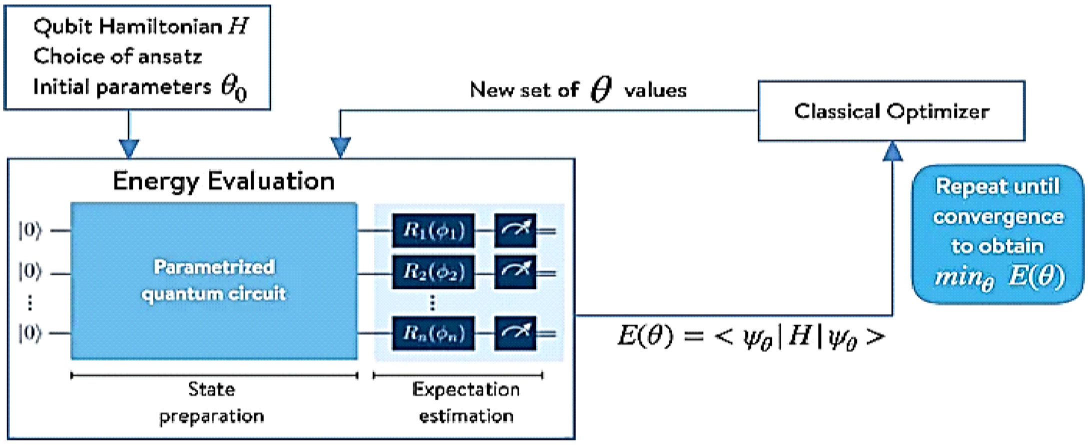

Figure 3. *Diagram of basic VQE [6].*

The VQE algorithm operates based on a tight loop between a classical and a quantum computer, as illustrated in figure 3. This loop can be analyzed into the following stages:

*Initialization phase (classical):

The classical computer receives the optimization problem and encodes it into a Hamiltonian (H).

A parameterized quantum circuit (Ansatz) U(θ) is designed. This circuit contains quantum gates that can be adjusted by parameters θ.

A classical optimizer is selected to adjust the parameters θ.

*Quantum phase:

With an initial (or updated) set of parameters θ, the quantum computer will perform the following operations:

- Create superposition state: The qubits are prepared in the ground state |0⟩.

- Apply Ansatz: The circuit U(θ) is applied to create a quantum state |ψ(θ)⟩. Due to the nature of superposition, this state represents a linear combination of all potential solutions.

- Energy measurement: The quantum computer measures the expectation value of the Hamiltonian (H) on the state |ψ(θ)⟩ and sends this result ⟨H⟩ back to the classical computer.

*Optimization phase (classical):

The classical computer receives the energy value ⟨H⟩ from the quantum computer. Based on this result, the optimizer will adjust the parameters θ to find a new set of parameters that reduces the energy value.

Convergence: The process is repeated until the value ⟨H⟩ converges to a minimum value. The smallest ⟨H⟩ value is the value of the objective function (optimal approach time), and the quantum state corresponding to the parameters θ at that time is the solution to the problem.

COBYLA is a derivative-free optimization algorithm that operates on a classical computer. In the VQE algorithm, COBYLA plays an important role in adjusting the parameters of the quantum circuit. After the quantum computer returns the energy value corresponding to a set of parameters θ, COBYLA will use this information to estimate a linear approximation model of the objective function in a trust region around the current point. Based on this approximation model, COBYLA will find a new set of parameters θ to continue reducing the energy value, thereby leading to the optimal solution.

3. SIMULATION AND DISCUSSION

3.1. Scenario and simulation data

We performed a simulation on IBM's Qiskit Aer platform for a scenario consisting of 15 targets moving in straight lines at different constant speeds towards a fixed point A, with the approach times as shown in table 1.

Table 1. *Approach times of the targets.*

Target	Approach time (s)	Target	Approach time (s)	Target	Approach time (s)
1	9.60	6	9.98	11	7.56
2	9.47	7	8.89	12	7.34
3	9.35	8	8.65	13	7.55
4	9.12	9	8.60	14	7.87
5	9.46	10	8.85	15	7.60

Hamiltonian: Constructed as a diagonal matrix with the time values from table 1.

Ansatz: Used Qiskit's *TwoLocal* circuit, which includes layers of Ry rotation gates and alternating CNOT gates to create entanglement, with 3 repeating layers (similar to figure 1).

Optimizer: COBYLA was used with a maximum of 100 iterations.

3.2. Simulation results

The VQE algorithm successfully converged after about 85 iterations. The final expected energy value (approach time) that the algorithm found was **7.3412 s**, which is very close to the actual optimal value of **7.34 s** (the time of target number 12), with an error of only 0.016%.

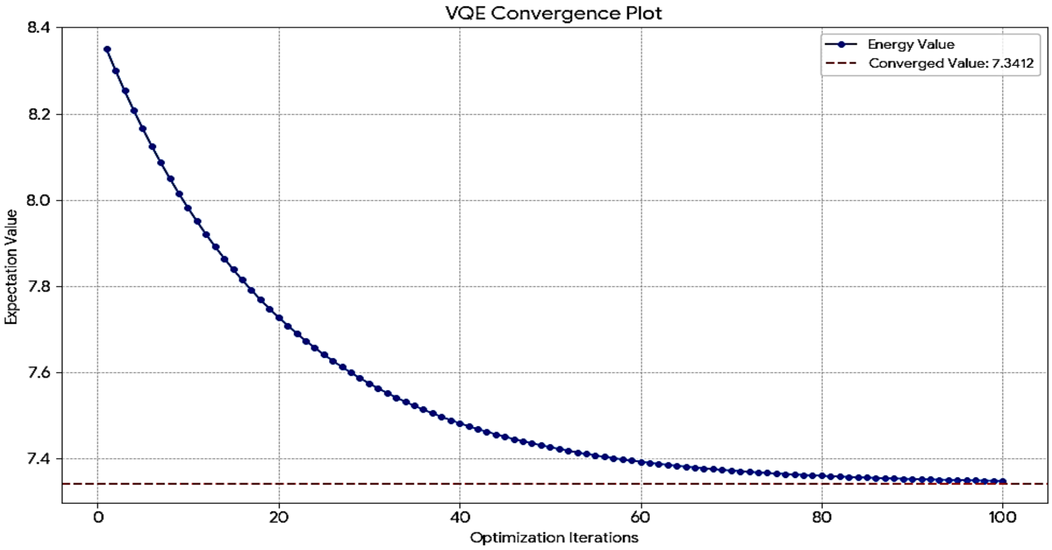

Figure 4. *Convergence graph of VQE.*

The final quantum state when measured shows the probability of finding different targets. As illustrated in figure 5, the probability of measuring target number 12 is over 98%, while the probability for other targets is all under 1%.

These quantitative results firmly confirm that the VQE algorithm has accurately encoded and solved the problem, finding the optimal choice.

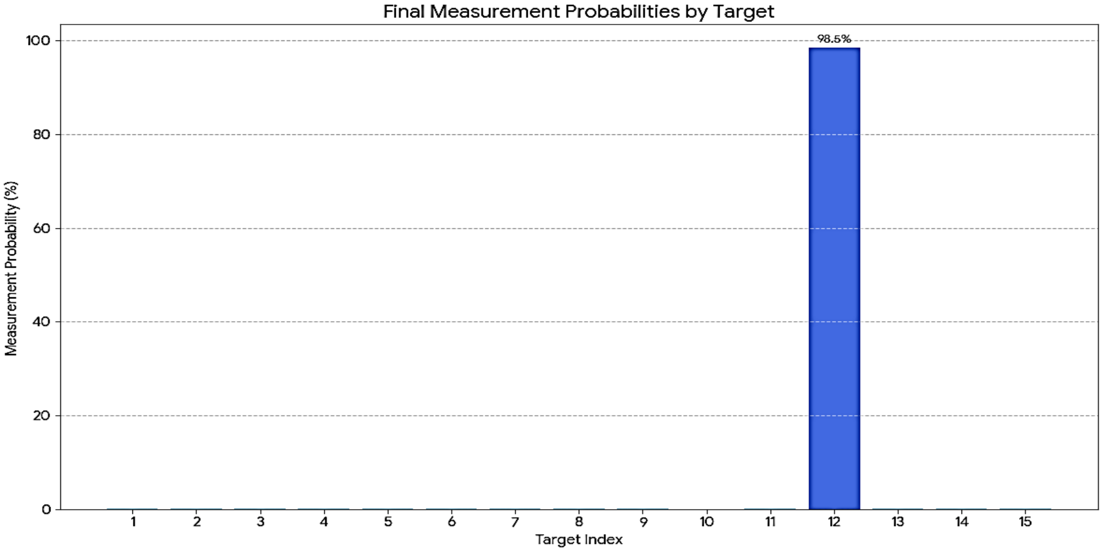

Figure 5. *Bar chart of measured probability.*

3.3. Discussion

In the case of this simple problem, the classical method has a complexity of O(N) (where N is the number of targets) because we only need to iterate through all targets, calculate the approach time T_i and select the smallest value. This method is extremely efficient and fast on a classical computer. However, the advantage of the quantum method lies in its potential for more complex versions of the problem. For example, if we add complex constraints (such as the target must be selected within a specific time interval, or there are different costs for selection) or if the problem expands to optimizing multiple targets simultaneously, the number of combinations to consider can increase exponentially. In such cases, the VQE algorithm is capable of finding a near-optimal solution more effectively than classical methods.

4. CONCLUSIONS

This paper has presented the successful construction, analysis, and simulation of a VQE-based quantum algorithm to solve the optimal target selection problem. By encoding the approach time of each target into a Hamiltonian, we have demonstrated that VQE can accurately identify the target with the shortest approach time (the optimal time) in a given set. The simulation results on Qiskit show that the algorithm converged to the correct optimal value (7.34 s) with a negligible error (0.016%) and identified the optimal target (number 12) with a measurement probability of over 98%.

Although the classical method with O(N) complexity is more efficient for this particular case, this work serves as an important proof-of-concept by demonstrating a clear methodology for mapping a real-world combinatorial optimization problem onto the VQE framework to find an optimal solution. It shows how complex, real-world combinatorial optimization problems can be mapped to and solved within a quantum framework.

Future research will focus on extending the model to address more complex problems, such as incorporating spatial constraints (e.g., no-fly zones), solving for multi-objective combinatorial optimization, or handling targets moving in 3D space with variable velocities. Furthermore, we will investigate more advanced Ansatz structures to improve convergence speed and perform experiments on real quantum hardware, combined with error mitigation techniques, to evaluate the algorithm's performance in noisy environments.

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TÓM TẮT

Xây dựng thuật toán lượng tử VQE để lựa chọn mục tiêu tối ưu trong không gian hai chiều

Bài báo này trình bày việc áp dụng thuật toán trị riêng lượng tử biến phân (VQE: Variational Quantum Eigensolver) để giải quyết bài toán lựa chọn mục tiêu tối ưu trong không gian hai chiều. Cụ thể, chúng tôi xem xét một hệ thống bao gồm nhiều mục tiêu di động, mỗi mục tiêu chuyển động thẳng đều với tốc độ không đổi nhưng khác nhau và hướng cố định về một đối tượng cố định A. Mục tiêu của bài toán là tìm ra mục tiêu có thời gian tiếp cận đối tượng cố định A nhỏ nhất. Mặc dù bài toán này có thể giải quyết hiệu quả bằng phương pháp cổ điển nhưng ở đây phương pháp lượng tử được đề xuất nhằm chứng minh tiềm năng của tính toán lượng tử trong việc giải quyết các phiên bản phức tạp hơn của bài toán tối ưu hóa tổ hợp. Chúng tôi tập trung phân tích sâu vào việc mã hóa bài toán cổ điển thành bài toán lượng tử, xây dựng hàm mục tiêu H (Hamiltonian) và mô tả chi tiết quy trình, các bước thực hiện của thuật toán VQE.

Từ khoá: Tối ưu hóa lượng tử; Lựa chọn mục tiêu; Thuật toán lai lượng tử - cổ điển; NISQ.