Analysis of NP and QMA Problems Energy Landscape Using Mutually Unbiased Bases

M.Sc. Research Proposal

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Abstract

In quantum mechanics, Mutually Unbiased Bases (MUB) are sets of quantum states that are maximally distinct from one another and exhibit a lack of information when a state from one basis is measured in another basis. These MUB represent a powerful tool for characterizing quantum states. Our primary objective is to demonstrate the utility of MUB in obtaining a reliable energy landscape for optimization problems. The energy landscape, as a tool for optimization, potentially plays a crucial role in efficiently identifying the global minimum solution while avoiding local minima and barren plateaus when dealing with problems (or cases) that are not NP-hard. Our secondary goal, regards the field of not NP-hard problems, is integrating the MUB approach with machine learning techniques to enhance the efficiency of the optimization process. This integration aims to reduce the number of search steps required to reach the optimal solution and represents a novel approach to the optimization of NP problems and QMA problems which can be modeled as quantum systems.

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1 Introduction and Background

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1.1 Mutually Unbiased Bases

Mutually unbiased bases (MUB) are a fundamental concept in quantum information that have been studied extensively in recent years. They are a set of orthonormal bases in a Hilbert space that are pairwise unbiased, meaning that the inner product between any two states from different bases is the same [1]. This property has important implications in quantum mechanics, including quantum state tomography and quantum error correction.

1.1.1 Mathematical Definition of MUB

The mathematical definition of mutually unbiased bases is given as follows: Let $B1$ and $B2$ be two orthonormal bases in a d-dimensional Hilbert space. $B1$ and $B2$ are said to be mutually unbiased if and only if the absolute value of the inner product between any two vectors in the two bases is equal to $\frac{1}{\sqrt{d}}$. Additionally, the existence of MUB in a d-dimensional Hilbert space has been proven to be linked to the mathematical structure of the unitary group and the finite Fourier transform over finite fields.

When the dimensionality ,d , of the Hilbert space is prime $d = p$ or power of prime $d = p^n$, it is possible to construct $d + 1$ MUB [1]. In addition, for certain composite dimensions, there exist subsets of MUB that satisfy certain conditions, such as the so-called "symmetric informationally complete positive operator-valued measures" (SIC-POVMs), which can be used in quantum state tomography and related applications.

1.1.2 Usages in Quantum Tomography

Recent research has focused on finding MUB in large-dimensional Hilbert spaces, as well as exploring their potential uses in quantum state tomography and quantum information science. Quantum state tomography is the process of learning an unknown quantum state from repeated state preparations and measurements, and yields optimal knowledge of the state's density matrix. MUB can be used to obtain this information efficiently, as they provide a way to obtain unbiased estimates of the density matrix elements. In particular, the use of symmetric informationally complete positive operator-valued measures (SIC-POVMs), which form a special subset of MUB, has been shown to provide accurate and efficient reconstructions of quantum states in a variety of contexts. For example, SIC-POVMs have been used in quantum process tomography to reconstruct the dynamics of

quantum channels, as well as in experimental studies of high-dimensional entanglement [2][3].

1.1.3 Usages in Quantum Cryptography

MUB have been proposed as a tool for quantum key distribution (QKD). In QKD, a key is shared between two parties in a secure way [?]. There are QKD protocols in higher dimensions, utilizing mutually unbiased bases (MUBs) and implemented through photons possessing orbital angular momentum [4]. The study employs (d+1) MUBs in both a classical preparation-measurement setup and with entangled photon pairs, across dimensions from d=2 to d=5. The analysis takes into account detection efficiency and the probability of photon pair creation. Key security metrics such as average error rate, shared mutual information between sender and receiver, and the rate of secret key generation per photon are derived from the experimental data. The results highlight that elevating the dimension can boost the information capacity and enhance the photon's key generation rate, with significant improvements observed up to a dimension of d=4. Another example is where the quantum cryptographic method by Bennett and Brassard can be expanded to use three conjugate bases, or six states, increasing security [?]. This method, using mutual information, offers better protection against single-qubit eavesdropping. Additionally, it explores the link between maximum classical correlation and the overlap of mutual information to enhance the cryptographic protocol.

1.2 Variational Quantum Algorithms (VQA)

Variational quantum algorithms (VQA) are a class of quantum algorithms that utilize a classical optimization loop to find the optimal parameters of a quantum circuit [5]. VQAs are designed to solve optimization problems and sample problems, including finding the ground state energy of a quantum system and solving linear systems of equations. One of the key features of VQAs is their ability to handle large quantum systems with a shallow quantum circuit.

1.2.1 Variational Quantum Eigensolver (VQE)

The Variational Quantum Eigensolver (VQE) is a popular and widely used VQA, designed to find the eigenvalues of a quantum Hamiltonian, which describes the energy of a quantum system. The VQE algorithm consists of a parameterized quantum circuit that is used to generate a wavefunction that approximates the ground state of the Hamiltonian. The circuit parameters are optimized using a classical optimization algorithm to minimize the energy expectation value of the wavefunction with respect to the Hamiltonian. This process is repeated until convergence, at which point the final wavefunction is used to estimate the ground state energy [6]. VQE has been applied to a wide range of problems

in quantum chemistry, including the calculation of molecular energies and properties, as well as the simulation of materials. In particular, VQE has been shown to be highly effective for simulating small and medium-sized quantum systems, where exact diagonalization and quantum Monte Carlo methods become infeasible due to the exponential scaling of the dimension of the quantum state space. Besides quantum chemistry, VQE has been used for a variety of applications, including optimization problems modeled by Ising-model Hamiltonians [7] [8]. The Ising model is a mathematical model used to describe the behavior of interacting spins in a system. The Ising-model Hamiltonian can be mapped onto a quantum circuit, which can then be optimized using VQE [7]. By finding the ground state of the Ising-model Hamiltonian, researchers can obtain an approximate solution to the original problem.

Another application of VQE is in solving systems of linear equations, where the goal is to find the solution to a set of linear equations. The fundamental state, or ground state, of a Hamiltonian can be used to solve linear equations in a way that is similar to classical linear algebra algorithms. Specifically, the Hamiltonian can be constructed such that its ground state corresponds to the solution of the linear equations. By finding the ground state of the Hamiltonian using VQE, the solution to the linear equations can be obtained [9]. One should underscore the fact that the term "E" in VQE, which stands for eigensolver, predominantly denotes an eigenvalue solver, primarily tasked with the identification of minimal energy level. Nevertheless, on occasion, it may also be employed to reference an eigenstate solver.

1.2.2 QAOA

The Quantum Approximate Optimization Algorithm (QAOA) is a VQA that was introduced in 2014 [10] to address combinatorial optimization problems. QAOA involves the construction of a parameterized quantum circuit, which is optimized using classical optimization algorithms to minimize a cost function related to the problem at hand. The cost function is formulated as a sum of Pauli products, and the QAOA circuit acts as a parameterized rotation of these products in the computational basis. The QAOA algorithm has been applied to various optimization problems, including MaxCut, Minimum Vertex Cover, and Max-SAT, among others, demonstrating its potential for solving combinatorial optimization problems on quantum computers. In MaxCut problem, the goal is to partition a graph into two sets such that the number of edges between the sets is maximized. The QAOA algorithm has also been shown to be effective for tackling optimization problems in classical machine learning and operations research, such as portfolio optimization and logistics planning.

1.3 Energy Landscape

An energy landscape is a concept used in physics and chemistry to describe the potential energy of a system as a function of its configuration or of its hamiltonian parameters [11]. The configuration of a system refers to the positions and orientations of its components. For example, in a protein, the configuration refers to the positions and orientations of its amino acids [12]. The energy landscape is often represented as a surface or a plot, with energy values on the vertical axis and the coordinates of the system's configuration on the horizontal axes [11]. The landscape can have different features such as minima, maxima, and saddle points, which correspond to stable, unstable, and meta-stable states of the system, respectively. A local minimum is a point on the energy landscape where the energy is lower than that of its immediate surroundings. It corresponds to a stable state of the system, meaning that small perturbations will not cause the system to move away from that point [11]. A global minimum is a point on the energy landscape that has the lowest energy of all possible configurations, and it represents the most stable state of the system [11]. The energy landscape is a useful concept for understanding the behavior of systems that can exist in multiple configurations, such as proteins, glasses, and phase transitions. It helps to visualize the possible configurations of the system and their relative stability. It is also used to design algorithms for finding the global minimum of the energy function [13].

1.3.1 Connecting VQE to Energy Landscape

The optimization algorithms tasked with selecting the successive parameters for the VQE do not offer a guarantee to bypass local minima or preclude entrapment within barren plateaus while conducting the search for the global minimum—the latter being the preferred solution. The application of energy landscape methodologies, in tandem with the use of MUB, could substantially enhance the probability of achieving the global minima. A comprehensive elucidation of this approach is available in the subsequent 'Objective of Research' section of this paper.

1.4 Vehicle Routing Problem

The Vehicle Routing Problem (VRP) is a central problem in the field of transportation and logistics. It aims to find the most efficient routes for a fleet of vehicles to visit a set of customers, typically referred to as "stops" or "delivery points", while minimizing the total distance traveled. Determining the optimal solution to VRP is NP-hard [14].

One of the most common NP-hard versions of the VRP is the Capacitated Vehicle Routing Problem (CVRP) [15]. In the CVRP, a fleet of vehicles with limited capacity must be used to serve a set of customers, each with a known demand. The objective is to minimize the

number of vehicles and the total distance traveled while satisfying the capacity constraints. Another common NP-hard version of the VRP is the Vehicle Routing Problem with Time Windows (VRPTW) [16]. In the VRPTW, each customer has a time window during which they can be serviced, and the objective is to minimize the total travel time while ensuring that all time windows are satisfied.

1.4.1 Classical Computing Approaches for the Solution

The Vehicle Routing Problem (VRP) has been extensively studied by researchers from various fields, including operations research, computer science, and mathematics. Researchers have proposed a wide range of solution methods for the VRP, including mathematical programming, heuristics, and meta-heuristics. There are several approaches that researchers have used to try and solve the VRP:

- Mathematical Programming: Researchers have tried to solve the VRP by formulating it as a mathematical programming problem and using various optimization algorithms to find the optimal solution. Due to the complexity of the problem, finding an exact optimal solution for large instances of the VRP is computationally infeasible. Therefore, researchers have developed various approximations and optimization algorithms to find near-optimal solutions. Some of the most common methods used to solve the VRP include linear programming, integer programming, and constraint programming [17]. e.g. constraint programming involves formulating the VRP as a set of constraints and using constraint satisfaction algorithms to find a feasible solution.
- Heuristics: Researchers have also developed heuristics and meta-heuristics, such as genetic algorithms, simulated annealing, tabu search, and ant colony optimization, to quickly find near-optimal solutions to the VRP.
- Artificial Intelligence: Researchers have also applied various artificial intelligence techniques, such as neural networks and decision trees, to find good solutions to the VRP.
- Exact Algorithms: Researchers have also developed exact algorithms, such as branch-and-cut and branch-and-price, to find the optimal solution to the VRP. These algorithms are typically exponentially slow but guarantee an optimal solution [18].
- Hybrid Approaches: Researchers have also combined multiple approaches, such as combining heuristics and exact algorithms, to find better solutions to the VRP [19].

All of these approaches have been successful to some extent in solving the VRP, but the VRP remains a challenging problem and there is still ongoing research in this area. The VRP is a complex problem that has many variations and applications, and researchers

continue to explore new approaches to solve it.

1.4.2 Quantum Computing Approaches for the Solution

One of the quantum computing approaches for solving the VRP is the quantum annealing algorithm. Innovative hybrid algorithms were developed, utilizing quantum annealing to tackle the Vehicle Routing Problem (VRP) and its Capacitated variant (CVRP). This study also introduced quantum-exclusive algorithms, with rigorous testing conducted via D-Wave's Leap framework. The outcomes indicate that these hybrid methods can provide competitive or potentially superior solutions compared to traditional algorithms for VRP and CVRP. [20].
In light of the aforementioned, it remains imperative to acknowledge that, as of the current state of research, a definitive conclusion regarding the superiority of D-Wave's quantum annealer over its classical counterpart has yet to be established.

Another approach is the quantum-inspired hardware, which mimic the behavior of quantum systems to solve similar optimization problems. This technology have been shown to be effective, more robust than heuristics,and more scalable than classical optimization solvers. [21].

There were VQE solution approaches for VRP [22]. Analysis of the effects of noise in a gate-based simulation of an algorithm to solve the vehicle routing problem. It was found that amplitude damping noise causes the least impact on the results of an optimized variational circuit. In contrast bit-phase-flip, depolarising and phase-flip noise channels had the maximum negative impact. One of the needed steps, of course was modeling VRP in qunatum, in other words mapping the cost function of VRP to an Ising Hamiltonian H_c,

$$H_{Ising} = -\sum_i \sum_{i<j} J_{ij} s_i s_j - \sum_i h_i s_i + d$$

$s_{ij} \in \{-1, 1\}$ is a spin variable which came up from binary decision variable $x_{ij} = (s_{ij} + 1)/2$. The terms J_{ij} ; h_i and d are defined as follows,

$$J_{ij} = -\frac{Q_{ij}}{2}, \forall i < j$$

$$h_i = \frac{g_i}{2} + \sum \frac{Q_{ij}}{4} + \sum \frac{Q_{ji}}{4}$$

$$d = c + \sum_i \frac{g_i}{2} + \sum_i \sum_j \frac{Q_{ij}}{4}$$

2 Related Work

There are few parers about using quantum annealing to solve those kind of optimization problems, that are intractable for classical computers. Quantum Annealing (QA) is a method for solving optimization problems that is inspired by the process of annealing in metallurgy. Like classical simulated annealing, it is a method that uses a random search to find the global minimum of an energy function, but it uses the principles of quantum mechanics to guide the search. In QA, the optimization problem is mapped to a physical system, called the quantum annealer, which consists of a large number of interacting quantum bits (qubits). The energy function of the optimization problem is encoded into the Hamiltonian of the quantum annealer, and the ground state of the Hamiltonian corresponds to the optimal solution of the problem.

The quantum annealer is initialized in a high-energy state, and then it is slowly cooled down to its ground state by applying a time-dependent Hamiltonian. The cooling process is guided by a schedule that controls the rate of change of the Hamiltonian. The schedule is designed to avoid getting stuck in local minima and to increase the chances of finding the global minimum.

3 Objectives of the Research

The purpose of the M.Sc. research is to configure a way to draw the energy landscape of a quantum system using MUB. Through that, a great number of realizations can be reached, for example avoid local minima and find the absolute minimum, avoid barren plateaus. In our research, we are going to focus on a problem which preoccupies the entire optimization world, the Vehicle Routing Problem. Although our research will focus on this problem as our quantum system, one can refer to other NP-hard problem, after the usage of MUB as a potential tool for drawing the energy landscape will be demonstrated. In the pursuit of our research objective, the utilization of quantum algorithmss and the implementation of a hybrid quantum-classical approach may provide significant benefits. In particular, the modeling of our problem into VQE or QAOA has the potential to offer improved approximations and the discovery of larger subclasses of NP-hard problems that are not NP-hard themselves.
Despite the limitations imposed by shallow quantum circuits, such a hybrid solution may still outperform traditional classical methods, providing a promising avenue for further exploration and advancement in the field. VRP can be modeled as a search for the global minimum of an energy function, when the energy function represents the cost of a particular solution, such as the total distance traveled by vehicles or the total time taken to visit all customers. The configuration space is defined by the possible routes and

the assignments of customers to vehicles. The global minimum of the energy function corresponds to the optimal solution of the problem.
The search in the energy space can be done by using machine learning model or neural networks, for the correct differential fluctuations needed in the angles of each quantum eigenstate of the mutually unbiased bases in use. The use of machine learning in the context of MUB is motivated by two main considerations. Firstly, the exponential growth of the number of MUB states for a large number of qubits necessitates the development of techniques for efficiently selecting a portion of these states or selecting them only for a subset of qubits. Secondly, even for small numbers of qubits, there is a need for innovative methods to explore the space beyond the vicinity of MUB states. This approach can significantly reduce the computational resources required for the VQE algorithm, making it more scalable for larger problems. We think about using MUB to construct energy landscapes of quantum systems using machine learning techniques. This can provide new insights into the behavior of the system that can be hard to gain by using other methods. The application of machine learning algorithms can help to overcome challenges by allowing for the characterization of smaller-scale problems and facilitating the transfer of insights to more complex systems with a larger number of qubits. In order to gain a comprehensive understanding of the landscape, it is necessary to not only examine the exact MUB-states points but also their surrounding regions. This can be achieved through two methods: By initiating the quantum circuit at each MUB state while incorporating a parametrized circuit that combines the MUB state with a standard ansatz. By starting at each MUB state and constructing a small-angle ansatz through the implementation of small-angle rotations of each qubit and small-angle rotations of the controlled-phase operation.

4 Other Research Directions

In addition to our main research topic, Prof. Mor and I are collaborating on other research problems. We plan to expand Qandies [23] [24] [25] terminology usage for explaining other quantum key distribution protocols and quantum phenomenas such as entanglement-swapping and delay-choice entanglement-swapping [26].

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