Entanglement and Quantum Algorithms: The QAOA Perspective

Submitted in partial fulfillment of the requirements
of the degree of

Bachelor of Technology
(Engineering Physics)

by

Aneesh Kamat
(Roll No. 200260006)

Supervisor:
Prof. Siddhartha Santra

Department of Physics
INDIAN INSTITUTE OF TECHNOLOGY BOMBAY
9th April 2023

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Date: 9th April 2023

Aneesh Anand Kamat

Roll No. 200260006

Abstract

Quantum technology has come a long way since Feynman's pioneering intuition that only a device inherently based on quantum mechanical principles could simulate nature [1]. A big question is whether such devices have the potential to establish "Quantum Supremacy" as discussed by Preskill [2].

Several quantum algorithms have been discovered, some addressing problems that were hitherto unsolvable and others introducing speed-ups on existing classical algorithms. The underlying idea driving such innovations is the use of novel quantum resources. The most celebrated example of a quantum resource is entanglement, thus an understanding of the role it plays in quantum algorithms is a fundamental necessity.

In the current regime of quantum devices - the NISQ era [3] - hybrid quantum-classical algorithms or Variational Quantum Algorithms (VQAs) are touted as the best strategy to outperform classical algorithms. The Quantum Approximate Optimization Algorithm (QAOA) [4] is a shallow-depth gate-model VQA designed to solve combinatorial optimization problems.

We consider the QAOA algorithm for solving the paradigmatic MaxCut problem on different families of three graph topologies - complete, bipartite complete and random - and examine the evolution of entanglement through continuous and discontinuous bipartite measures. We investigate the feasibility of classically simulating the QAOA and the scaling of the algorithm with problem size and circuit depth by analyzing the evolution of entanglement through the algorithm.

We further explore the behaviour of entanglement at the phase transition of 1/2 edge-to-node ratio for random graphs, below which efficient classical algorithms exist to solve the MaxCut. In this context, we discuss the possibility of obtaining a quantum advantage using QAOA.

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List of Abbreviations

BP	Barren Plateau
COBYLA	Constrained Optimization BY Linear Approximations
MPS	Matrix Product States
MaxCut	Maximum Cut
NISQ	Noisy Intermediate-Scale Quantum
VQA	Variational Quantum Algorithm
QAOA	Quantum Approximate Optimization Algorithm

Chapter 1

Introduction

Quantum computation and quantum information are the study of information processing tasks that can be accomplished using quantum mechanical systems. Feynman envisioned quantum computing as he fundamentally believed quantum mechanics to be difficult to simulate using classical computation, thus the push for a new paradigm that reimagines computation at its fundamentals and builds a model that is inherently designed to address quantum mechanical questions. Quantum computation's much touted computational speed-up or "quantum advantage" is built on the consideration that it can tap into quantum resources [7], a set of resources beyond the classical computational resources.

As one of the integral features of quantum mechanics, entanglement presents one such essential quantum resource. One can use quantum entanglement to explore the capabilities of several families of algorithms that try to understand the properties of quantum many-body states. An entanglement-inspired vantage point also enables one to define the boundary between systems that can be simulated classically and those that need quantum machines and simulators for an accurate description. The role of entanglement in pure state quantum computation has been studied extensively [**?** 8, 9, 10]. Several insightful results from this pursuit motivate our work and are duly highlighted below.

First, it has been shown that quantum computations can be classically simulated efficiently if the amount of entanglement (using appropriate measures) is bounded such that it does not scale unfavourably with the dimension of the Hilbert space of the computation [**?**]. Second, it is known that even some highly entangled quantum computations can be efficiently simulated classically [9]. In these two cases therefore there can be no quantum-computational advantage. Third, it has also been demonstrated that teleportation is a universal quantum primitive [10] which implies that entanglement in the form of pure Bell-states is sufficient for quantum computation.

Fourth, it has been shown by Maarten Nest [8] that a vanishing amount of entanglement - in terms of continuous measures of entanglement such as entanglement entropy but not in terms of discrete measures such as the Schmidt-rank entanglement - is sufficient for universal quantum computation.

The upshot of the first three of these results is that entanglement during the evolution of a computational algorithm is considered to be a necessary but not a sufficient indicator of the possible quantum advantage provided by an algorithm. The crucial export of the fourth result is that the measure of entanglement also has to be appropriately chosen.

Quantum advantage can be said to be achieved when a quantum computer outperforms a classical one at a specific problem in speed, size or quality. One needs a simulator to run quantum circuits classically and the tools necessary can be categorized into two types - exact (state vectors, Feynman paths, and tensor networks) and approximate (matrix product states (MPS) [**?**], projected entanglement pair states, tree-tensor networks).

Amongst these, MPS are perhaps the best-established simulation tools and the effect of χ, known as the bond dimension, on the properties of a quantum state represented by MPS are well documented. The bond dimension is a measure of the entanglement in the system and relates to the von Neumann entanglement entropy as $S \sim ln\chi$.

Quantum supremacy through QAOA has been explored from a complexity theory perspective [11] and it has been shown that efficient sampling from the output of even the lowest depth version $(p = 1)$ of this algorithm would collapse the polynomial hierarchy (a tower of classes of problems which seemingly require more and more resources to solve). Here, we investigate the potential for a quantum advantage in QAOA through the lens of entanglement evolution,

and note the scope for the extension of this pursuit to VQAs and universal quantum algorithms in general.

This report is organized as follows. First we review the role of entanglement in quantum computation and outline some relevant theoretical and analytical constructs that will be used later to justify our analysis. We describe the onset and motivation behind VQAs in general and QAOA in particular before moving on to briefly discuss the barren plateau issue and account for our choice of optimizer. We discuss the paradigmatic Maximum Cut (MaxCut) problem and rationalize our choice of graph families for the analysis. We then present our hypothesis, and outline our strategy and methodology using the tools we have introduced. This leads to an analysis of the entanglement generated during QAOA as a factor of the circuit depth, model size and graph family. We conclude with a discussion on the potential extension of this approach to VQAs in general and the implications similar results could carry.

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Chapter 2

Background

Now, we shall outline some building blocks for our analysis and review some relevant literature to develop our argument.

2.1 Role of Entanglement in Quantum Computing

To motivate our work, let us begin with a discussion on the role of entanglement in quantum computing. One fundamental non-classical feature of quantum formalism is the rule for how the state space S_{AB} of a composite system AB is constructed from the state spaces S_A and S_B of the parts A and B. In classical theory, S_{AB} is the Cartesian product of S_A and S_B, whereas in quantum theory it is the tensor product (and the state spaces are linear spaces).

This essential distinction between Cartesian and tensor products is precisely the phenomenon of quantum entanglement, namely the existence of pure states of a composite system that are not product states of the parts. It has been comprehensively put forward that the phenomenon of entanglement is responsible for an essential difference in the complexity (as quantified below) of physical evolution allowed by the laws of quantum physics in contrast to

that allowed by the laws of classical physics. [12]

There are two primary arguments to draw a relationship between entanglement and the apparent ability of a quantum process to perform a computational task with exponentially reduced resources (compared with any classical process).

The first concerns the physical resources needed to represent superpositions in quantum versus classical theory. The second concerns the classical computational cost of mimicking a typical step in quantum computation. Jozsa concludes on qualitative grounds that if a quantum algorithm (on pure states) is to offer an exponential speed-up over classical algorithms, then entanglement must appear in the states used by the quantum algorithm.

Another result from their paper is that for any quantum algorithm operating on pure states, the presence of multi-partite entanglement, with a number of parties that increases unboundedly with input size, is necessary if the quantum algorithm is to offer an exponential speed-up over classical computation.

In summary, the point is that we can have different mathematical formalisms for expressing quantum theory and, although they are fully mathematically equivalent, they will lead to quite different families of states (of increasingly many qubits) that have a polynomially sized description with respect to the chosen formalism. Hence, we also get different notions of a physical quality that guarantees a state will not be of the latter form. Then every one of these qualities must be present in a quantum algorithm if it is to offer an exponential speed-up over classical algorithms.

Vidal showed, that if at all times, under any bipartite cut, the state of the quantum computer has Schmidt-rank entanglement polynomial in n, then the computation can be efficiently classically simulated. In other words, to give an exponential speedup the quantum algorithm needs to achieve Schmidt-rank entanglement of exponential order in n, during computation.

That the presence of entanglement is only necessary but not sufficient for exponential quantum speedup follows from the Knill-Gottesman theorem [10]. It states that operations from the Clifford group composed with Pauli measurement in a computational basis can be efficiently simulated on a classical computer. This class of operations can, however, produce highly entangled states. For this reason, and as indicated by others, the role of entanglement is still not clear. As it is pointed out by Jozsa [13] it may be that what is essential for quan-

tum computation is not entanglement but the fact that the set of states which can occur during computation cannot be described with a small number of parameters.

As outlined in the introduction, Vidal, Gottesman and Maarten have made substantial arguments to indicate that entanglement during the evolution of a computational algorithm is considered to be a necessary but not a sufficient indicator of the possible quantum advantage provided by an algorithm.

2.2 Measures of Entanglement

In classical systems, one uses entropy to quantify the lack of knowledge of the state of the system due to thermal fluctuations. However, for a quantum system at zero temperature, the entropy of a subsystem has a different origin: entanglement.

The fundamental question in quantum entanglement theory is which states are entangled and which are not. Only in a few cases does this question have a simple answer. The simplest is the case of pure bipartite states. Any bipartite pure state $|\Psi_{AB}\rangle \in \mathscr{H}_{AB} = \mathscr{H}_A \bigotimes \mathscr{H}_B$ is called separable (entangled) if and only if it can (cannot) be written as a product of two vectors corresponding to Hilbert spaces of subsystems:

$$|\Psi_{AB}\rangle = |\phi_A\rangle|\psi_B\rangle.$$

2.2.1 Continuous and Discrete Measures

To quantify and analyse the entanglement, we use two bipartite entanglement measures - the von Neumann entropy and the Schmidt-rank entanglement, which are continuous and discrete measures of entanglement, respectively.

All composite pure states can be partitioned into two subsystems A and B. We obtain the reduced density matrix ρ_A by tracing out subsystem B,

$$\rho_A(|\Psi\rangle) = \mathrm{Tr}_B(|\Psi\rangle\langle\Psi|),$$

The von Neumann entropy generalizes the concept of Shannon entropy to quantum states and is given by $S(\rho_A) = -(\rho_A \log \rho_A)$.

The Schmidt-rank entanglement is equal to the rank of the reduced density matrix. It is defined through the Schmidt decomposition:

$$|\Psi\rangle = \sum_i \lambda_i |i_A\rangle i_B\rangle,$$

where the bases $|i_A\rangle$ and $|i_B\rangle$ are called the Schmidt bases for A and B, respectively, and the number of non-zero values λ_i is called the Schmidt number for the state $|\Psi\rangle$.

2.2.2 VQAs and QAOA

One of the main advantages of VQAs is that they provide a general framework that can be used to solve a variety of problems. Although this versatility translates into different algorithmic structures with different levels of complexity, there are basic elements that most (if not all) VQAs have in common. In this section, we review the building blocks of VQAs.

The first step to developing a VQA is to define a cost (or loss) function C which encodes the solution to the problem. One then proposes an ansatz, that is, a quantum operation depending on a set of continuous or discrete parameters θ that can be optimized. This ansatz is then trained in a hybrid quantum-classical loop to solve the optimization task.

The trademark of VQAs is that they use a quantum computer to estimate the cost function $C(\theta)$ (or its gradient) while leveraging the power of classical optimizers to train the parameters θ. They potentially offer computational capabilities beyond the best classical computers and algorithms available currently by leveraging the domains of both the classical and quantum

computing realms. An excellent review of VQAs is available by Cerezo et al [6].

The Quantum Approximate Optimization Algorithm (QAOA) was originally introduced to obtain approximate solutions for combinatorial optimization problems [4]. The ansatz used in QAOA involves an alternating structure and is often called the quantum alternating operator ansatz [14], sharing the same acronym as the algorithm (although we will use QAOA to refer to the algorithm here). This ansatz was first shown to be computationally universal for certain Hamiltonians in [15], with the proof of its universality being generalized in [16] for families of ansatzes defined by sets of graphs and hyper-graphs.

We now describe the algorithm, QAOA starts with a uniform superposition over the n bitstring basis states,

$$|s\rangle = |+\rangle^{\otimes n} = \frac{1}{2^n} \sum_{z \in \{0,1\}^n} |z\rangle.$$

Then, choosing $2p$ variational parameters $(\vec{\gamma}, \vec{\beta}) = (\gamma_1, \ldots, \gamma_p, \beta_1, \ldots, \beta_p)$, a variational state is obtained through $2p$ evolutions applied to the initial state

$$|\vec{\gamma}, \vec{\beta}\rangle = U(H^B, \beta_p) U(H^C, \gamma_p) \ldots U(H^B, \beta_1) U(H^C, \gamma_1) |s\rangle,$$

where the evolution operators are defined as

$$U(H^C, \gamma) = e^{-i\gamma H^C} = \prod_{\alpha=1}^{m} e^{-i\gamma H^C_\alpha}, U(H^B, \beta) = e^{-i\beta H^B} = \prod_{j=1}^{m} e^{-i\beta H^B_j}$$

with $H^B = \sum_{j=1}^{n} X_j$ as the *mixing Hamiltonian*.

This demonstrates the impressive scope of the QAOA using low-depth circuits made of simple elements such as single-qubit Pauli X's and two-local ZZ Hamiltonians on a one-

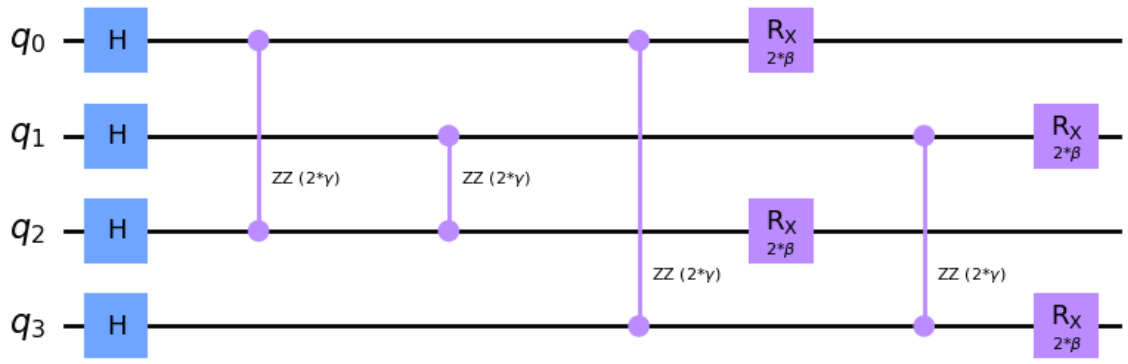


Figure 2.1: A simple demonstration for MaxCut on a 4-node graph using QAOA with one layer $(p = 1)$.

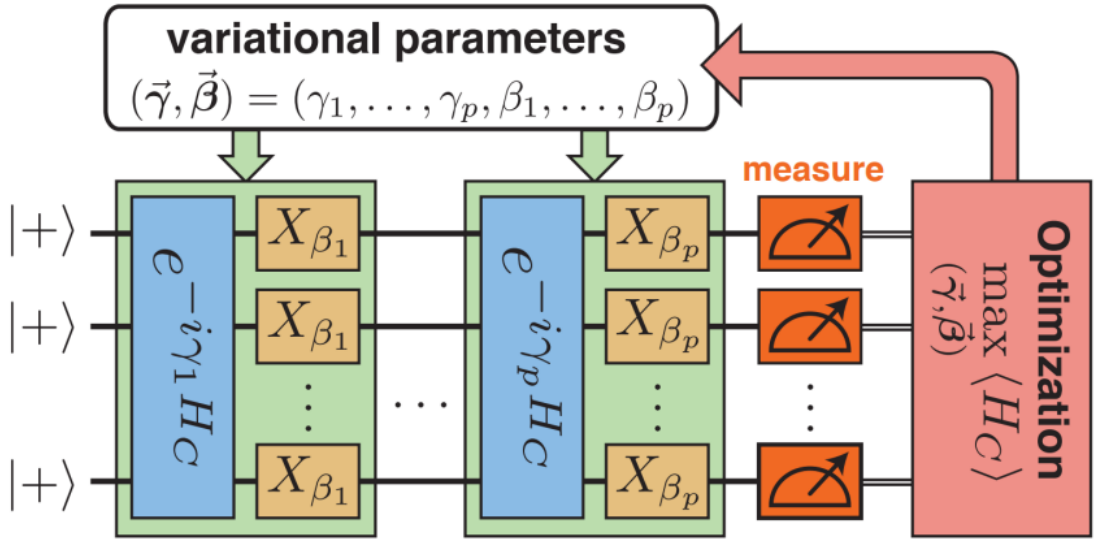


Figure 2.2: Schematic of a p-level QAOA. [5]

dimensional line of qubits. Hence, QAOA is particularly well suited for applications in the NISQ era with a goal to obtain states via a feedback procedure during each iteration of which an objective function is minimised with respect to certain circuit parameters.

2.2.3 Barren Plateaus and COBYLA

The barren plateau (BP) phenomenon in the cost function landscape has received considerable attention as one of the main bottlenecks for VQAs. When a given cost function $C(\theta)$ exhibits a BP, the magnitude of its partial derivatives will be, on average, exponentially vanishing with the system size. The exponential scaling in the precision due to BPs could erase a potential quantum advantage with a VQA, as its complexity would be comparable to the exponential scaling typically associated with classical algorithms. Hand-in-hand with the theoretical progress in the analysis of the BP phenomenon, great effort has been dedicated to avoiding or mitigating the effect of BPs. The main strategy here has been to break the assumptions leading to BPs. In what follows we present two main approaches [6]: parameters initialization and choice of ansatz. We also rationalize our choice of optimizer for the simulator.

2.2.3.1 Parameter Initialization

Randomly initializing an ansatz can lead to the algorithm starting far from the solution, near a local minimum, or even in a region with BPs. Hence, optimally choosing the seed for θ at the beginning of the optimization is an important task. The importance of parameter initialization was made clear in [5] where it was noted that the optimal parameters in QAOA exhibit persistent patterns. Based on these observations initialization strategies were proposed and which were heuristically shown to outperform randomly initialized optimizations. Here, we explore the parameter space for the chosen problem and graph family and heuristically choose an initialization of 1.0 for every (γ_i, β_i).

2.2.3.2 Ansatz Strategies

Another strategy for preventing BPs is using structured ansatzes which are problem-inspired. The goal here is to restrict the space explored by the ansatz during the optimization. As discussed in the section on ansatzes, the quantum alternating operator ansatz for optimization are problem-inspired ansatzes which are usually trainable even when randomly initialized. One of the strengths of this ansatz is the fact that the feasible subspace for certain problems is smaller than the full Hilbert space, and this restriction has the potential to result in a better-performing

algorithm.

2.2.3.3 COBYLA Algorithm

Our choice of the optimization algorithm is motivated by Brandhofer's analysis of implementing QAOA on classical optimizers [17]. The COBYLA method is a derivative-free optimization algorithm that is well-suited for optimizing functions that are not smooth or have discontinuities. It stands for "Constrained Optimization BY Linear Approximations" and works by iteratively constructing linear approximations of the objective function and performing a constrained optimization on each approximation.

It is a robust gradient-free optimization method which is preferable for simulations in IBM's 'qasm simulator', where the sampling noise prevents a precise evaluation of the gradient. This includes the measurement process which, for a finite number of shots (in our case: 2048), leads to a statistical sampling error due to the random measurement outcomes. Several optimizers were considered, but COBYLA proved the most consistent at small p.

2.3 MaxCut Problem

MaxCut is an NP-hard optimization problem that looks for an optimal 'cut' for a graph $G(V,E)$ in the sense that the cut generates a subset of nodes $S \subset V$ that shares the largest amount of edges with its complement $V \setminus S$. In a slightly modified form (omitting the constant), it has the following objective function

$$\max_s \frac{1}{2} \sum_{\langle i,j \rangle \in E} 1 - s_i s_j \ ,$$
$$s$$

where the $s_i \in \{-1,1\}$ are the variables and i, j are the edge indices. This function can be easily converted into an Ising cost Hamiltonian, which takes the form

$$H_C = \frac{1}{2} \sum_{\langle i,j \rangle \in E} I - Z_i Z_j.$$

We consider the standard mixing Hamiltonian that sums over all nodes:

$$H_M = \sum_{v \in V} X_v.$$

As the initial state $|\Psi_0\rangle$ we take the uniform superposition, given by

$$|\Psi_0|\rangle = \frac{1}{\sqrt{2^{|V|}}} \sum_{x=0}^{2^{|V|}-1} |x\rangle$$

2.4 Graph Families

In the context of the MaxCut problem, different topologies of graphs can be used to test the performance of algorithms under different conditions, such as the density of the graph, the distribution of edge weights, or the structure of the subgraphs. Ultimately, the choice of topology will depend on the specific problem at hand and the algorithm being used to solve it. For our analysis we consider three topologies:

2.4.1 Complete Bipartite Graphs

This family of graphs is intuitively fundamental for bipartition-based analysis for the MaxCut problem as the central cut is trivially the best choice to maximise the cut, as the system is already partitioned into two sets such that the number of edges crossing a central partition is

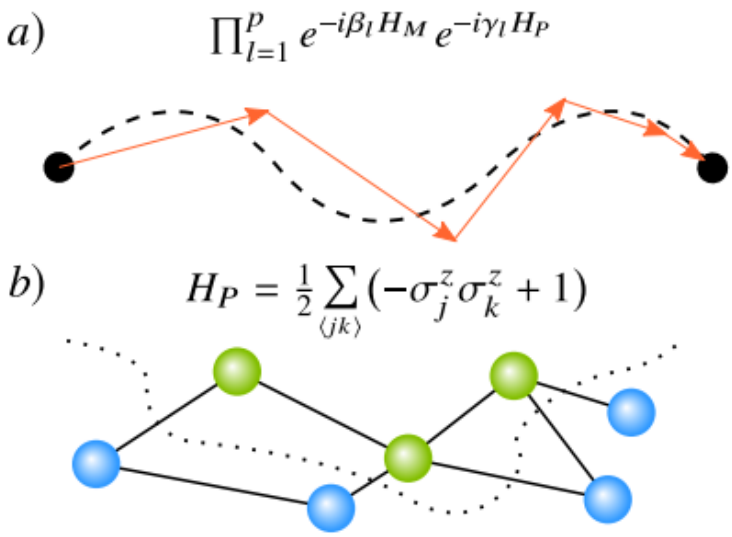


Figure 2.3: a) Schematic drawing of the Trotterized adiabatic transformation in the ansatz. b) Problem Hamiltonian HP and graph $< jk >$ for a Max-Cut task. Each node in the graph (circle) represents a spin. Vertices connecting two nodes indicate an interaction $\sigma_j^z \sigma_k^z$ in H_P, with σ_k^z the Pauli z operator on spin k. The solution is encoded in the ground state of H_P where some spins are pointing up (green) whereas others point down (blue). [6]

maximized. Our analysis for this topology acts as a reference for more complicated problems. We take 4, 6 and 8-node cases.

2.4.2 Complete Graphs

The most general and basic family of graphs for the MaxCut problem is the family of Complete Graphs. This is because a Complete Graph is a graph where every pair of vertices is connected by an edge, which means that any other graph can be obtained from a Complete Graph by adding or removing edges.

In other words, the Complete Graph represents the most general and complete connectivity pattern between vertices. It provides the highest level of symmetry and regularity among all graphs and is often used as a benchmark for measuring the performance of algorithms that solve the MaxCut problem. We take 4, 6 and 8-node cases.

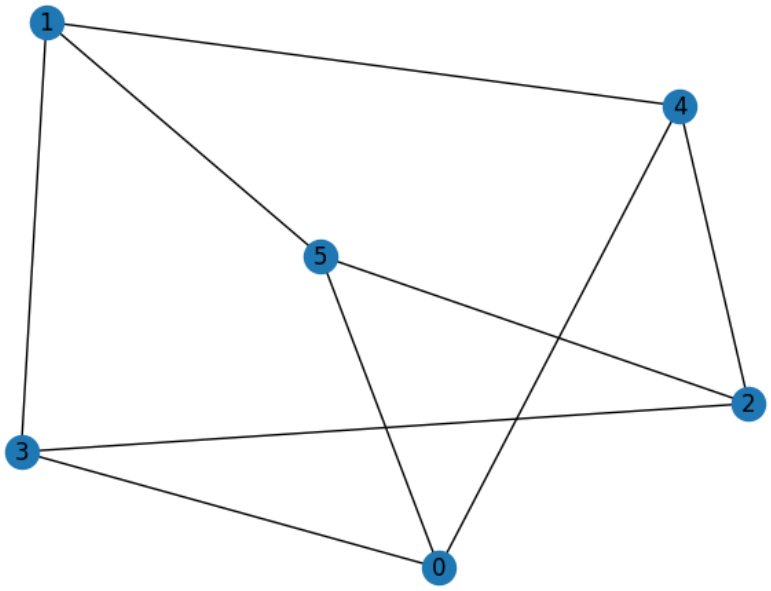


Figure 2.4: A 6-node bipartite complete graph. Note that the labels 0,1,2 are not connected with each other but are individually connected to all of the labels 3,4,5.

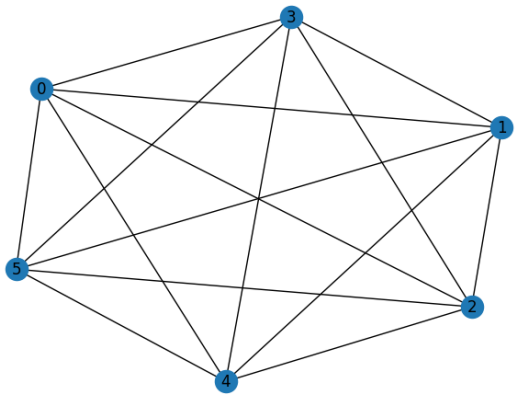


Figure 2.5: A 6-node complete graph. Note that every node is connected to each other.

2.4.3 Random Graphs

In this work, we generate random *Erdős–Rényi* graphs using the NetworkX package [18] for our MaxCut problem instances. The graphs are constructed following the $G(n,m)$ model, with n the number of vertices and m the number of edges.

We investigate the MaxCut at the complexity phase transition at the 1/2 edge-to-node ratio,

below which one finds efficient classical algorithms for solving the problem [19]. We consider 6, 8 and 10-node cases.

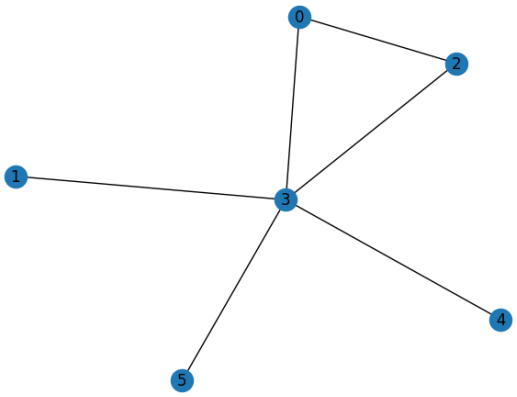


Figure 2.6: A 6-node random graph with 6 edges. Note that it is possible to have isolated nodes or clusters in sparse graphs with less edges.

Chapter 3

Hypothesis and Strategy

3.1 Hypothesis

In classical optimization problems, the target states do not intrinsically require a finite amount of entanglement. This makes such problems great testing grounds for studying whether the existence of entanglement helps accelerate the optimization process.

Our work investigates the hypothesis that even if the target state entanglement grows favourably with 'n' it can be so that intermediate steps in the computation, that is, at certain circuit depths the entanglement grows rather large with 'n'. In this case, classical simulation of the circuit will not be efficient along with the possibility of obtaining some quantum advantage via QAOA.

We postulate that the favourable or unfavourable growth of entanglement is dependent on the nature of the entanglement measure considered. Entanglement as measured by a continuous measure such as entanglement entropy does not grow unfavourably with the model size, but it does grow unfavourably with model size if measured by a discrete measure such as Schmidt-rank entanglement. [8] We intuit that, as the system size increases, growing amounts

of entanglement should be generated in order for a quantum algorithm to achieve an exponential quantum speed-up, Schmidt-rank entanglement in particular. [20]

We discuss the role of connectivity in graphs and the entanglement and complexity associated with it in the context of the QAOA applied to the MaxCut problem for bipartite complete and complete graphs.

We investigate a correlation between the classical hardness and quantum hardness for the MaxCut on the *Erdős–Rényi* random graphs with a 1/2 edge-to-node ratio, below which one finds efficient classical algorithms for solving the problem. [19]

3.2 Strategy

We consider an unweighted MaxCut problem on graph families of 2 topologies - Bipartite Complete and Complete graphs for 4, 6 and 8 nodes optimized by a QAOA circuit with the number of layers varying from 1 to 8. The qubits are initialized in the $|+\rangle$ state. The initial parameters for θ are fixed at 1.0 on the basis of a heuristic initialization discussed in Section 2.2.3.1 and a COBYLA optimizer is used to iteratively improve the QAOA parameters as introduced in Section 2.2.3.3.

We consider a central bipartition of the system (e.g. for 4 nodes, q[0] and q[1] are A, q[2] and q[3] are B) and calculate the Schmidt-rank entanglement and von Neumann entanglement entropy across the bipartition for every iteration, thus examining the evolution of entanglement throughout the algorithm. We also plot the expected cut value at convergence versus the depth of the circuit.

We then consider Random graphs of 6, 8 and 10 nodes and vary the edge connectivity in small steps. The QAOA is again initialized with 1.0 for all parameters and sample analysis of 10 and 100 randomly selected graphs for each edge number are considered. The statistical averages of the bipartite entanglement are plotted against the edge number to gauge the behaviour of entanglement at the complexity phase transition.

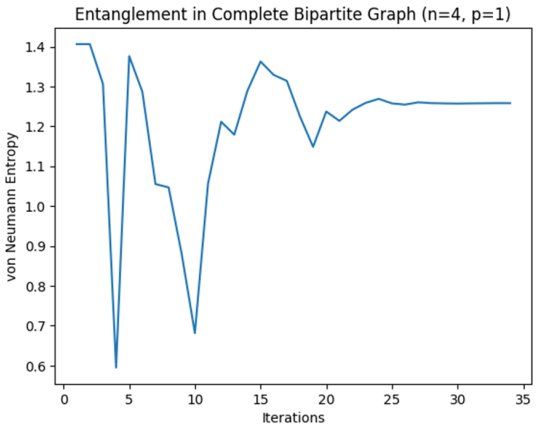
Chapter 4

Results and Analysis

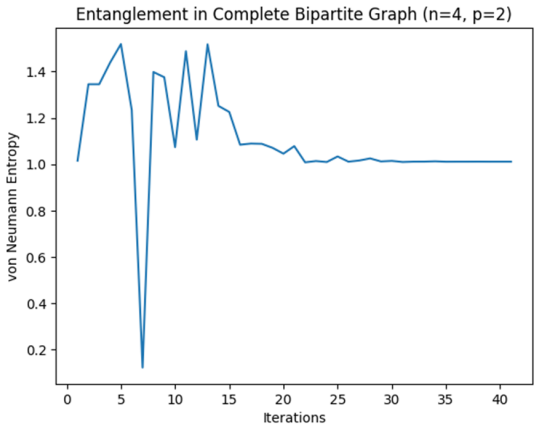
Our analysis demonstrated the growth of entanglement entropy in the intermediate stages of the QAOA algorithm even at a low depth and small model sizes, thus validating our first hypothesis that despite the output state of a classical optimization problem being a low-entangled superposition of a few bitstrings solving the optimization problem of interest, there is a significant role played by entanglement in between the initial and final low-entangled states.

A surprising output that contradicts our second postulate that the discrete measure of entanglement should grow unfavourably with model size, is that the Schmidt number behaves extraordinarily benignly for well-ordered topologies like the bipartite and complete graphs. It has a constant value for a particular model size, independent of whether the topology is bipartite complete or complete.

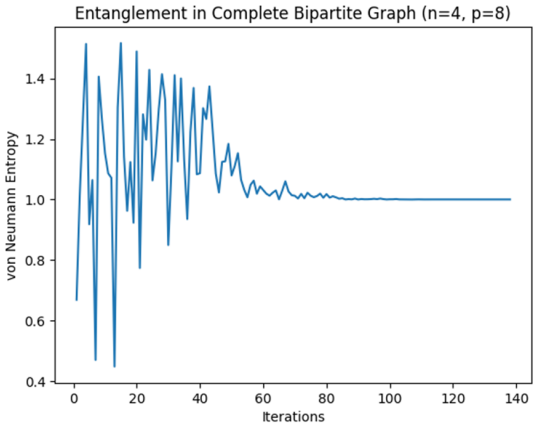
Now, we investigate the bipartite entanglement of the convergence state for the MaxCut on a random sampling of *Erdős–Rényi* graphs with 6, 8 and 10 nodes. Due to computational limitations, we average over 10 and 100 samples for 6-node graphs, but only over 10 samples for 8 and 10-node graphs.



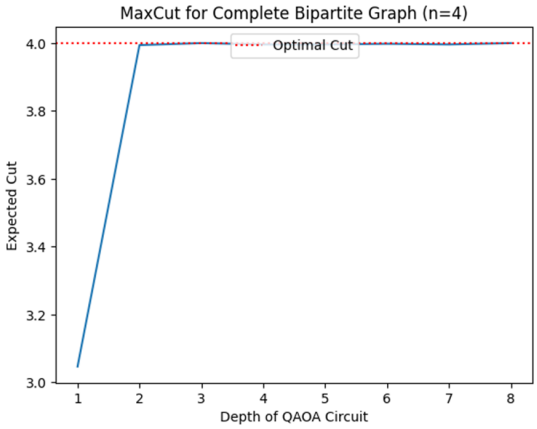
(a) For 1 layer.



(b) For 2 layers.

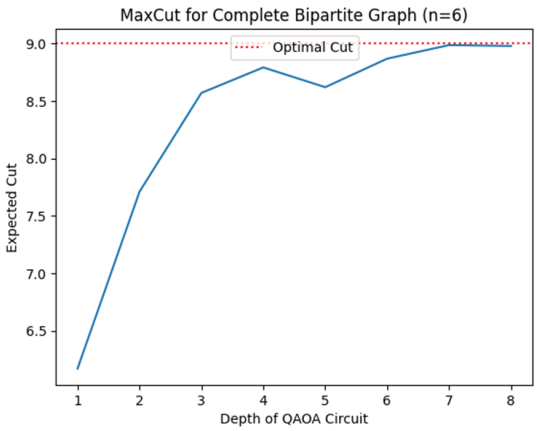


(c) For 8 layers.

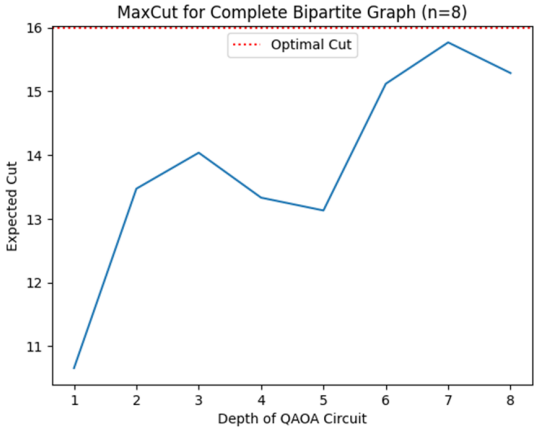


(d) Expected cut as a function of layers.

Figure 4.1: a,b,c) Dynamics of von Neumann entanglement entropy for a complete bipartite graph with 4 nodes and a Schmidt-rank entanglement of 3. d) Expected cut versus the depth of QAOA circuit. Observe how it converges to a very good solution within just one layer.

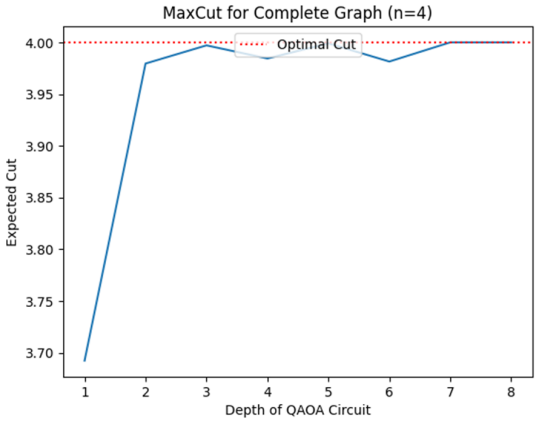


(a) For 6 nodes, Schmidt number = 4.

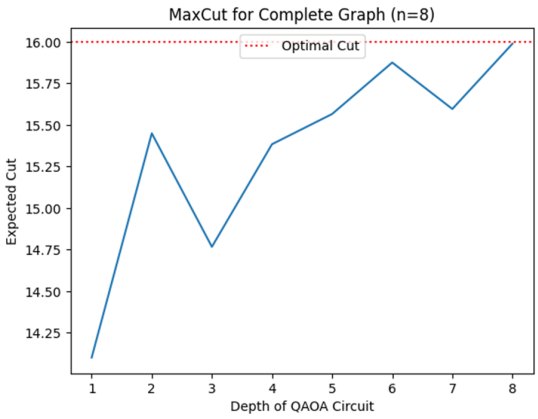


(b) For 8 nodes, Schmidt number = 5.

Figure 4.2: The growth of the expected cut as the depth of the circuit increases for 6 and 8 node bipartite complete graphs with Schmidt-rank entanglement of 4 and 5, respectively.

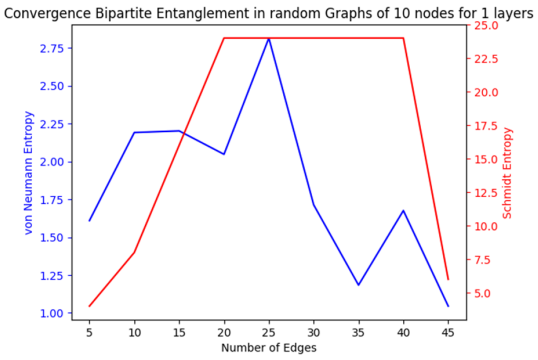


(a) For 4 nodes, Schmidt number = 3.

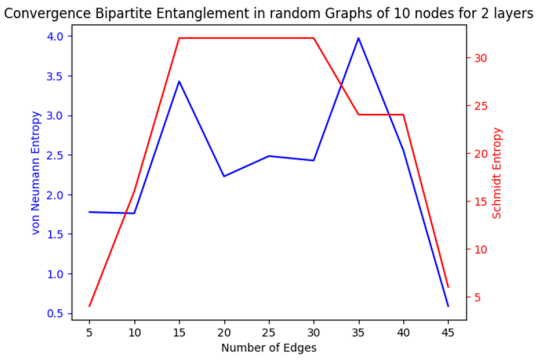


(b) For 8 nodes, Schmidt number = 5.

Figure 4.3: The growth of the expected cut as the depth of the circuit increases for 4 and 8-node complete graphs with Schmidt-rank entanglement of 3 and 5, respectively.

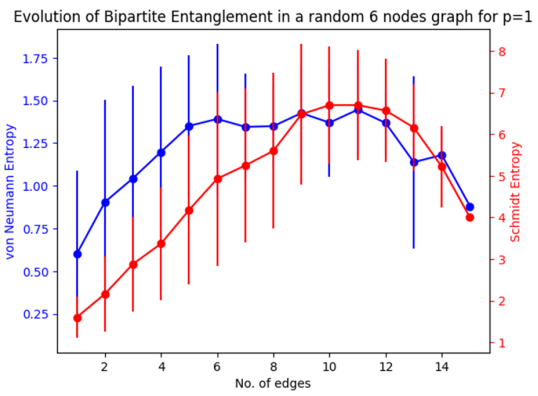


(a) For p=1 layer.

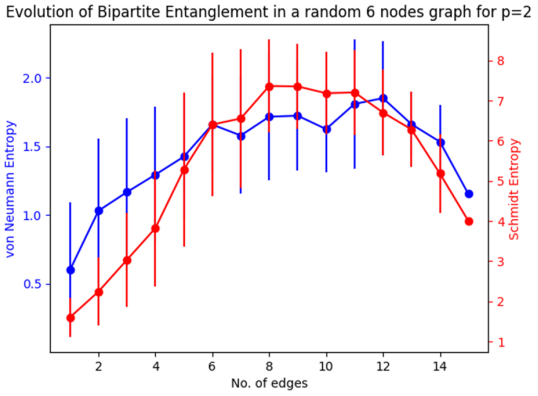


(b) For p=2 layers.

Figure 4.4: We randomly sample 10-node graphs for edge numbers varying from 5 to 45 in steps of 5 and plot the convergence bipartite entanglement.



(a) For p=1 layer.



(b) For p=2 layers.

Figure 4.5: We randomly sample 100 6-node graphs for edge numbers varying from 1 to 15 in steps of 1 and plot the convergence bipartite entanglement.

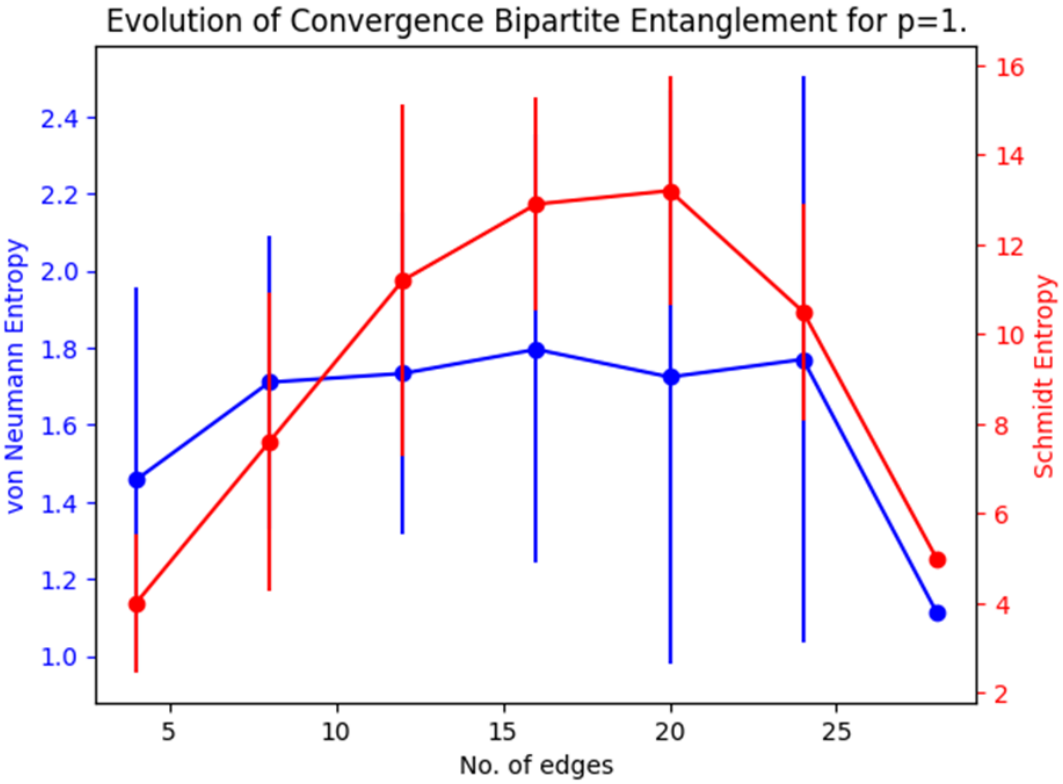


Figure 4.6: For p=1 layer and 10 random 8-node graphs with edge numbers varying from 4 to 28 in steps of 4.

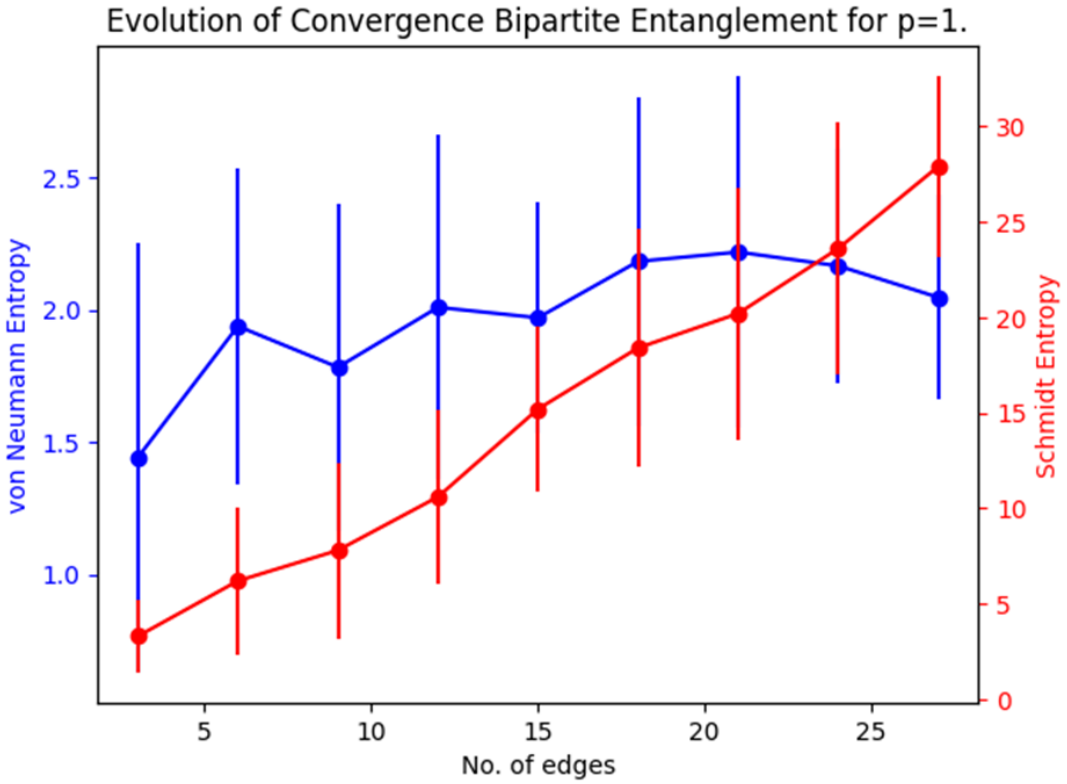


Figure 4.7: For p=1 layer and 10 random 10-node graphs with edge numbers varying from 5 to 45 in steps of 5, however, the algorithm couldn't converge beyond 30 edges.

Chapter 5

Conclusion and Open Questions

We conclude that bipartite entanglement behaves very differently under continuous and discrete measures for the QAOA on MaxCut problems. The continuous von Neumann entanglement entropy is quite dynamic and sensitive to parameters like problem size, circuit depth, and connectivity however it doesn't scale unfavourably to the extent that it highlights a difficulty in classically simulating the algorithm. The discrete Schmidt-rank entanglement, however, is only influenced by the problem size for complete and bipartite complete graphs and behaves in a strangely benign manner.

We observe that increasing the circuit depth increases the time to convergence and the fluctuations in von Neumann entropy. In general, more layers also improve the quality of the solution which can be gauged by the value of the expected cut and its distance from the Maximum Cut. For maximum connectivity, the case of the complete graph for 4, 6 and 8 nodes highlights that shallow circuits suffice to give good results, however, an increase in problem size necessitates an increase in depth.

In the case of Random graphs, we observe a distinct high-valued region near half-connectivity for both von Neumann and Schmidt-rank entanglement. Computational limitations prevent a thorough scaling analysis, but there is a pronounced peak for the 6-node case averaged over

100 samples. For the 8-node case, an analysis of the edge number in step of 4 was necessary to keep computational times reasonable, and the Schmidt-rank entanglement is observed to rise significantly. For the 10-node case, our algorithm fails to converge beyond 30 edges, however, this highlights the difficulty of the problem. We highlight that the Schmidt-rank entanglement increases monotonically up to this point before the suspected complexity phase transition.

In summary, we have identified the disparate behaviour of continuous and discrete bipartite entanglement measures for the QAOA applied on the MaxCut. For well-connected topologies, shallow circuits can be implemented to solve the MaxCut problem using the QAOA, for a general random graph, however, the connectivity influences the complexity and we note a correlation with the rise in the discrete bipartite entanglement for hard problems.

Further work can be directed along a few paths. A primary objective would be to explore the optimization landscape by randomly initializing the QAOA for various problems and observing the role of entanglement in searching the parameter space. Conducting a scaling analysis for problem sizes in the 50-100 node range would confirm the behaviour of discrete bipartite entanglement at the phase transitions. An implementation of this analysis on an actual quantum device as well as attempting to solve the same problems using the best classical solutions available would provide a crucial comparison. The analysis of the random graphs highlights the presence of particular cases that are difficult, categorizing these instances and observing some structure to problems that are difficult would provide crucial insights into areas where a quantum advantage could be explored.

Recent work in this area includes an analysis of the bipartite von Neumann entropy and the entanglement spectrum for randomized QAOA circuits and optimized QAOA circuits for the MaxCut problem on linear, 3-regular and complete graphs [21]. An investigation into the weighted MaxCut problem with a modified QAOA that requires lesser entanglement [22]. An MPS based simulation approach to QAOA with restricted entanglement and high circuit depth for the unweighted MaxCut on Erdos–Renyi graphs [23].

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Acknowledgments

I wish to record a deep sense of gratitude to **Prof. Siddhartha Santra**, my supervisor for his valuable guidance and constant support over the last 6 months and throughout my B.Tech project and related research. His approachability, responsiveness, and mentorship are crucial inputs to my enthusiasm in research.