Transferring Optimal QAOA Parameters Between Regular Graphs for Larger Circuit Depth

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Abstract

The Quantum approximate optimization algorithm (QAOA) is a quantum algorithm that aims to produce approximate solutions for combinatorial optimization problems. The quantum circuit parameters of QAOA are optimized to find the optimal solution. Recent research found that, for the Max-cut problem, the optimal parameters of the QAOA circuit for one graph with small number of nodes can be used for another graph with larger number of nodes if their degrees have the same parity. In this paper, we come up with the conjecture of the condition of parameter transfer for larger circuit Depth QAOA, and numerically verify it for regular graphs.

I. Introduction

At the end of the 19th century, it was found that classical theories could not explain microscopic systems. Then through the efforts of physicists, quantum mechanics was created in the early 20th century to explain these phenomena. As the investigation progressed, a lot of theories and mathematical tools were built by many famous scientists. Though, we still do not fully comprehend the quantum nature of reality. Applications based on quantum mechanical laws, such as quantum computing and other quantum technologies have developed in the last 20 years.

Quantum computing is the study of the information processing tasks that can be accomplished using quantum mechanical systems. Quantum computing has been shown to solve problems that are hard to be solved with a classical computer. A typical example is Shor's algorithm [6] which is a polynomial-time quantum computer algorithm for integer factorization. Furthermore, in 2014, the quantum approximate optimization algorithm (QAOA) was proposed by Farhi et al. [2] for solving the classically NP-hard combinatorial optimization problems, such as the Max-cut problem.

QAOA is a quantum-classical hybrid algorithm that the quantum circuits are constructed based on the set of variable parameters $\vec{\gamma}$ and $\vec{\beta}$. And these parameters are optimized with a classical optimizer for the highest energy quantum states, Recently, it is proven for low depth QAOA circuits on 3-regular graphs that fixed parameters could be used for other instances that come from some reasonable distribution [1]. Then, Galda et al. analyze the transferability of parameters between two graphs [3]. They summed up some laws of parameter transferring in the case of depth 1.

In this work, we find that for general graphs, when the depth of QAOA circuits exceeds 1, the number of cases of subgraphs goes vast. It is hard to demonstrate or verify the rules which determine the transferability quality. We do some experiments of parameter transferring and come up with some conjectures which are presented in Section IV. In the next section, we introduce some back-

ground of the QAOA and Max-cut problem. In section III, we summarize previous work on parameter transfer.

II. QAOA

The Max-cut problem is to cut the nodes of a graph into two sets and make the edges between the nodes form the two sets as many as possible. The classical objective function of Max-cut problems can be written as:

$$C(z) = \frac{1}{2}\sum_{j,k\in E}(1-(-1)^{z_j}(-1)^{z_k}) \tag{1}$$

where $z = z_1 z_1 \dots z_n$ is the bit string, E is the set of edges in the graph. The target of Max-cut problems is finding the bit string that maximizes the objective function. The bit string z is mapped as the basis vectors $|z\rangle$ of a 2^n dimensional Hilbert space in QAOA. The objective is converted into a diagonal Hamiltonian C that each basis state corresponds to an eigenstate. The Hamiltonian of the Max-cut problem is constructed as:

$$C = \frac{1}{2}\sum_{j,k\in E}(I - Z_j Z_k) \tag{2}$$

where Z_j and Z_k are the Pauli Z operators which act on j^{th} and k^{th} qubits. In this way, $C(z) = C|z\rangle$.

The QAOA circuit prepares a parameterized state of the form:

$$\begin{aligned}|\psi(\vec{\beta},\vec{\gamma})\rangle = U_B(\beta_p)U_C(\gamma_p)\dots \\ U_B(\beta_1)U_C(\gamma_1)H^{\otimes n}|0\rangle\end{aligned} \tag{3}$$

where $U_C(\gamma) = e^{-i\gamma C}$, $U_B(\beta) = e^{-i\beta B}$, $B = \sum_{j=1}^{n}\sigma^x$ the mixer Hamiltonian. H the operator to prepare the initial state $\frac{1}{\sqrt{2^n}}\sum_z |z\rangle$, and p is the layer number of QAOA circuits which also which is also known as depth. The objective function can be rewritten as:

$$F_p(\vec{\beta},\vec{\gamma}) = \langle\psi(\vec{\beta},\vec{\gamma})|C|\psi(\vec{\beta},\vec{\gamma})\rangle \tag{4}$$

We can find the optimal parameters ($\vec{\beta}$ and $\vec{\gamma}$) using a classical optimizer such that objective function $F_p(\vec{\beta},\vec{\gamma})$ is maximized.

III. Parameter Transfer

For the Max-cut problem, the objective function Eq.4 can be written in the following form:

$$\begin{aligned}F_p(\vec{\beta},\vec{\gamma}) &= \langle\psi(\vec{\beta},\vec{\gamma})|C|\psi(\vec{\beta},\vec{\gamma})\rangle \\ &= \frac{1}{2}\langle\psi(\vec{\beta},\vec{\gamma})|\sum_{j,k\in E}(I - Z_j Z_k)|\psi(\vec{\beta},\vec{\gamma})\rangle \\ &= \frac{|E|}{2} - \frac{1}{2}\sum_{j,k\in E}\langle\psi(\vec{\beta},\vec{\gamma})|Z_j Z_k|\psi(\vec{\beta},\vec{\gamma})\rangle \\ &= \frac{|E|}{2} - \frac{1}{2}\sum_{j,k\in E} f_{jk}\end{aligned}$$

The f_{jk} can be seen as an individual edge contribution to the total objective function. Because f_{jk} is local to only two qubits, most of the gates in the circuit cancel out. The circuit with the remaining gates that have not been eliminated can be seen as the QAOA circuit of the subgraph. These subgraphs include the edges whose distance to node j and k is less than p.

Brandao et al. [1] found that, if the 3-regular graphs are large enough, the subgraphs corresponding to most of the edges are the same. Therefore, the parameters of QAOA circuits could be fixed in this case. Inspired by this research, Galda et al. [3] come up with a strategy that optimizes the QAOA for a small graph which is called donor, then uses the donor's parameters for a large graph, called the acceptor. This process is known as parameter transfer. If the donor's parameters maximize the objective function of the acceptor's, it is a successful optimal parameter transferability. They studied the conditions that optimized parameters for one graph could also maximize the QAOA objective function for another graph.

Galda et al. focus on the $p = 1$ case. They found good transferability of parameters was in even-to-even and odd-to-odd subgraphs. For the general random graph, they did parameter transfer experiments between 55 subgraphs with the maximum degree less than or equal to 6. The results show that

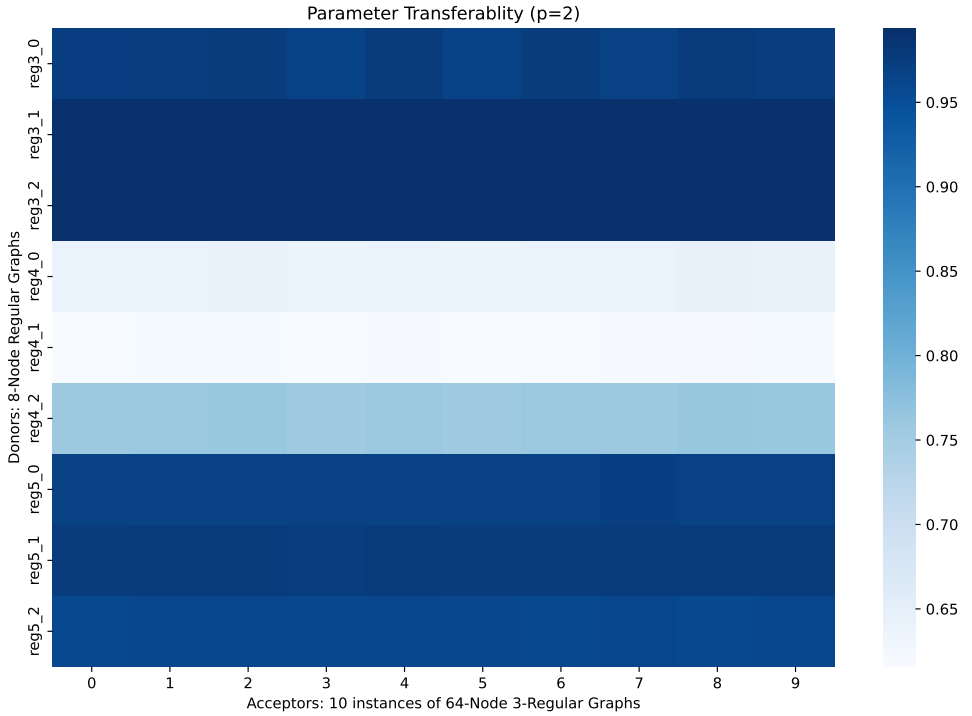


Figure 1: *Transferability map between 8-node 3- 4- 5- regular graphs and 64-node 3-regular graphs. Deeper blue represents better transferability . 3- and 5- regular graph donors show better transferability than 4- regular graph donors for 3-regular graph acceptors.*

when the degrees of node j and k are both odd or both even, the parameters of its subgraph show a good transferability for the subgraphs with the same characteristic. Also, it works well between the subgraphs with mixed degrees.

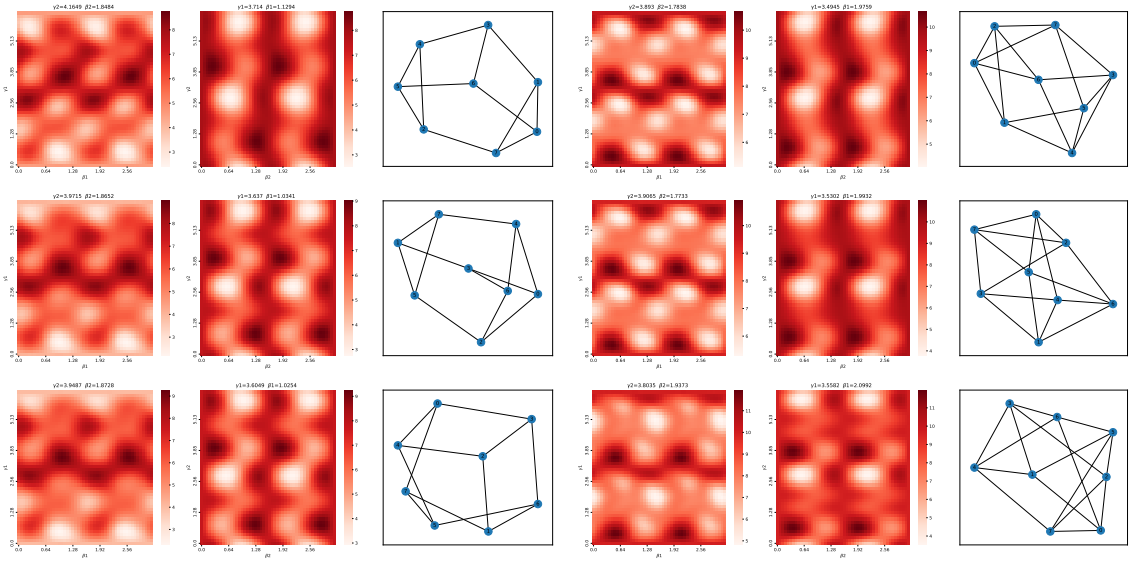
IV. Experiments

Based on the results from [3], we conjecture that optimized parameters can be successfully between regular random graphs which have the same parity when p exceeds 1. We do a brief series of experiments to verify this conjecture. We randomly generate 8-node 3- 4- 5-regular graphs of 3 each as donors, and 10 64-node 3-regular graphs as acceptors. We set p as 2, and transfer the parameter from donors to acceptors.

i. Details of Implementation

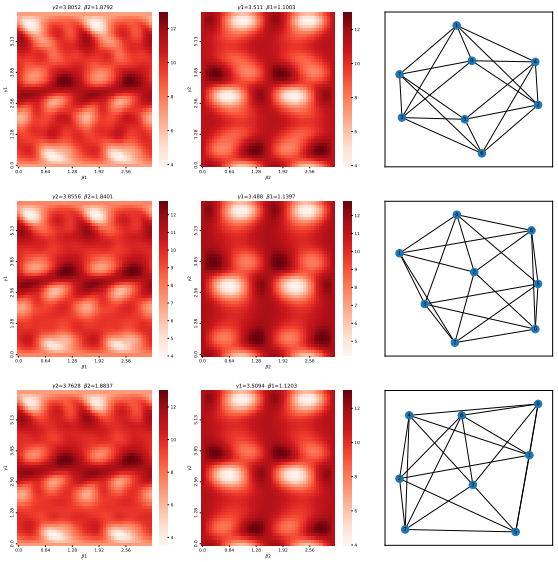
For the simulation of QAOA circuits, we consider that, from the classical perspective, QAOA consists of tensor calculations. This is like some deep learning models, such as Convolutional Neural Network. Usually, GPU is used for accelerating computing for these deep learning models. Inspired by this, we use PyTorch [5] which is a widely used deep learning framework to help to use GPU easily to simulate the QAOA. We use an RTX 3080 Ti graphic card which has 12 Gigabytes VRAM that allows us to simulate 14 qubits. Coincidentally, the largest subgraph of the graph whose max degree is 3 includes 14 nodes when p equals 2. Consequently, we could simulate QAOA for large 3-regular random graphs.

For the classical part of QAOA, we choose to use the Nelder-Mead method [4], an algo-

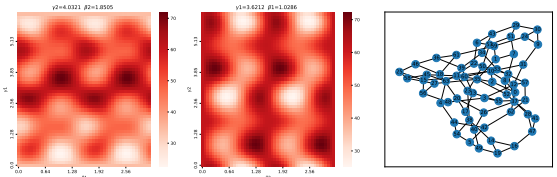


(a) Landscapes of Three 8-Node 3-Regular Graphs

(b) Landscapes of Three 8-Node 4-Regular Graphs



(c) Landscapes of Three 8-Node 5-Regular Graphs



(d) Landscape of One 64-Node 3-Regular Graph

Figure 2: *Landscapes. Deeper red represents the higher energy of the prepared states.*

rithm for finding the minimum or maximum of an objective function in a multidimensional space, which has the advantage of not requiring a derivable function and converging to a local minimum relatively quickly.

In addition, we found that there are multiple close optimized expected values that correspond to different sets of parameters for one graph when p exceeds 1. For the ease of analysis, we fix the initial value of the parameters to get similar optimized parameters.

ii. Results and Analysis

In this work, we use the transferability ratio $\frac{F_p(\vec{\beta}^\sharp,\vec{\gamma}^\sharp)}{F_p(\vec{\beta}^*,\vec{\gamma}^*)}$ ($\vec{\beta}^\sharp$ and $\vec{\gamma}^\sharp$ are donor's optimized parameters) to evaluate the quality of the transferability.

As shown in Fig. 1, parameters from 3- and 5- regular graph donors work well on the 3-regular graph acceptors, which is in line with our expectations.

Since the parameter set is in a high-dimensional space when p is greater than 1, it is difficult to visualize the landscape. For this reason, we change one set of γ and β of the optimized parameters and fix the rest of the parameters to get landscapes Fig.2. We can see the maxima position of 8-node 3- 5- regular graphs and 64-node regular graphs are very close. This explains why the parameter transfer is successful. Meanwhile, 4- regular graphs show different contributions, which further validates our conjecture.

V. Conclusion and Future Work

In this paper, we show that the parameter transfer still has a good performance when p equals 2. Therefore, the conjecture about parameter transfer in regular graphs also applies to the case when p exceeds 1.

In the future, we will work on the parameter transfer between the general random graphs. As shown in Table 1. when p exceeds 1, the number of kinds of subgraphs goes massive. Meanwhile, the subgraphs' node number will go beyond common classical computers' simulation capacity. We think it will be a challenge to find or verify some parameter transfer laws for general random graphs with larger p.

Table 1: *Number of Subgraphs*

	p		
Max Degree	1	2	3
2	3	5	6
3	9	527	
4	19		

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