Predicting Transferability of Parameters of Quantum Approximate Optimization Algorithm

Introduction

Are quantum computers of any use? Granted, these devices use intrinsic properties of quantum mechanics to solve problems where our current *classical* computers fall short. But general-purpose quantum computers are still decades away. In the meantime, can we use near term quantum devices for practical purposes, despite their limited resources?

One such avenue is graph optimization which is relevant not only for modeling epidemics like COVID-19 [1] but also containing their spread [2]. Using limited quantum resources, the Quantum Approximate Optimization Algorithm (QAOA) [3] has great potential for outperforming classical state-of-the-art methods in solving such problems. To speed up QAOA calculations, one promising technique reuses solutions of small graphs to solve larger graphs. However, computing such transferability remains a challenge. Therefore, I developed and tested multiple metrics which predict the transferability between random graphs.

Background

Consider a graph G in which vertices represent people and edges represent friendships between them. MaxCut, a graph optimization problem, aims to group strangers together and set friends apart. It does so by dividing the vertices/people into two groups such that the number of edges/friendships between the two groups is maximized.

QAOA employs both quantum and classical computers to solve this problem. It involves a classical optimizer which guesses parameters γ, β. These parameters determine the arrangement of people into the two groups. The quantum machine then computes such arrangement and returns the number of friendships across the partition or the energy of the graph, $G(\gamma, \beta)$, back to the optimizer. These back and forth exchanges occur until the algorithm converges to the maximum energy solution.

Transferability reduces the number of such exchanges in QAOA. In this technique, for an acceptor graph A, one finds a donor graph D whose optimal parameters γ_D, β_D also optimize the energy of the acceptor. The donor may be a smaller 'lower-cost' graph or a graph whose optimal parameters have already been computed. The success of transferability is defined as the degree to which donor's optimal parameters maximize the acceptor's energy, or

$$T(D, A) \equiv \frac{A(\gamma_D, \beta_D)}{A(\gamma_A, \beta_A)} \tag{1}$$

. However, this coefficient assumes one already knows the acceptor's optimal parameters γ_A, β_A when transferability, itself, is the means through which one finds them. As a result, this coefficient cannot be computed.

But we can still predict transferability. To do so, I addressed a deeper question: What makes two graphs share the same optimal parameters? The answer lay in the previous work done by my collaborators on regular graphs [4]. Generalizing their findings for random graphs, I tested whether graphs of similar parity share the same optimal parameters. Here, I defined parity of a graph as its *even-ness* or the proportion of its vertices with even number of edges. If the parity of a graph influences its optimal parameters, then I can use it to predict transferability between graph pairs.

Methods

To test the relationship between parity and optimal parameters, I analyzed the QAOA solution spaces of random graphs. I generated 110 distinct 20-node graphs, varying in parity, from the NetworkX Python Library

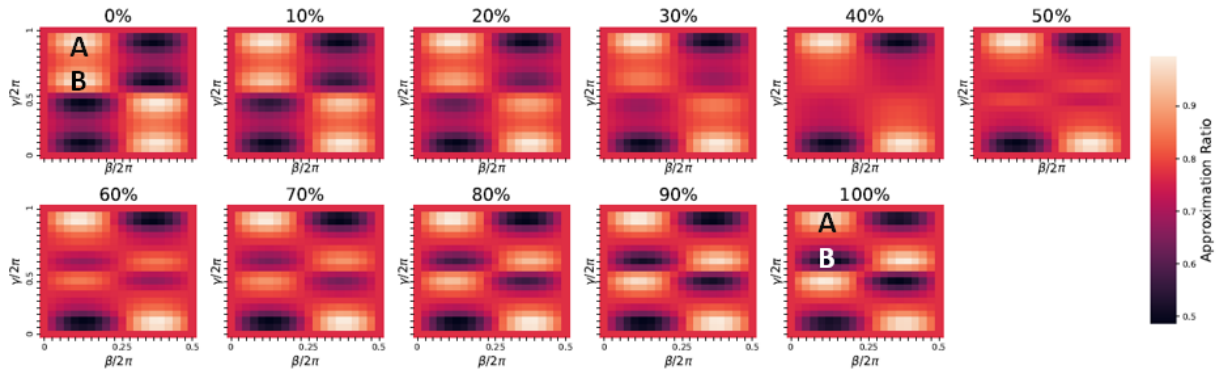

Figure 1: Energy landscapes of twenty node graphs sorted by parity. Each subplot is the average energy landscape of 10 distinct 20-node random graphs with the specified parity (% of vertices with even number of edges). Bright regions indicate maxima and dark regions indicate minima.

and computed their optimal parameters using the QTensor [5] simulator. Through the latter task, I built upon my existing skills in 2 crucial domains: quantum simulation and parameter optimization. First, for simulating quantum computers, I previously operated with large matrices, scaling exponentially with the resources of the system. In contrast, QTensor reduces the size of such matrices using tensor contraction algorithms, easing the simulation burden. Second, for optimizing the parameters, I used Root Mean Square Propagation , a popular machine learning algorithm which accelerates the traditional gradient descent method by dampening unwanted oscillations on the parameter space. Armed with these new tools, I efficiently optimized the graphs and generated the following results.

Results

Figure 1 reveals special features of QAOA energy landscapes of 20-node random graphs:

1. Two sets of parameters, one of which is labeled A in Figure 1, maximized the energy of all the random graphs, regardless of their parity. These are universal parameters.
2. Certain parameters maximize or minimize the energy of graphs based on their parity. For example, point B in Figure 1 is a maxima for odd graphs ($0-20\%$), but it gradually fades to become a minima for even graphs ($80-100\%$). These are non-universal parameters.

These features hold important consequences for transferability. After running QAOA on the donor graph, if its computed optimal parameters are universal like A, then its parameters are transferable to any acceptor in the dataset. However, if those parameters are non-universal like B, then the donor's parameters will be transferable only to acceptors which share similar parity. Hence, for the same graph pair, we could report radically different transferability coefficients depending on the computed optimal parameters of the donor. To avoid such inconsistencies, I redefined the transferability coefficient to average the energy contributions of *multiple* optimal parameters of the donor as

$$T'(D,A) = \frac{1}{N}\sum_{i=1}^{N}\frac{\mathsf{A}(\gamma_{D_i},\beta_{D_i})}{\mathsf{A}(\gamma_A,\beta_A)}, \qquad (2)$$

where $(\gamma_{D_i},\beta_{D_i})$ are the i'th set of the donor's computed optimal parameters. In this work, we chose $N = 20$ for convenience.

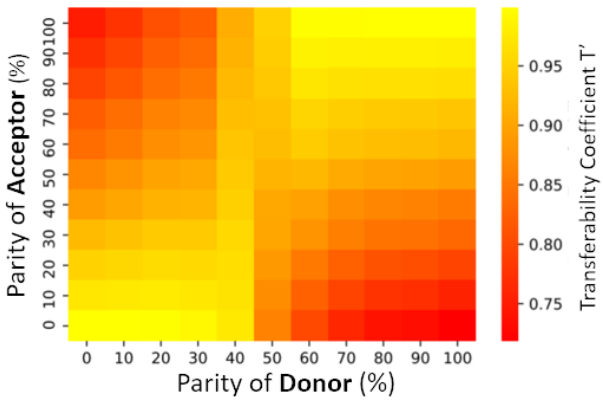

Figure 2: Transferability between 20-node random graphs, sorted by their parity. Each block represents the transferability coefficient averaged over 100 graphs pairs, constructed from 10 distinct donors and 10 distinct acceptors.

Observations from Figure 1 also provided support for my hypothesis that the parity of random graphs affects their transferability. To further test this claim, I computed the redefined transferability coefficient T' for the graph pairs in my dataset and the results are shown in Figure 2. As shown in the upper-right and the lower-left regions of the heatmap, even graphs and odd graphs transfer well amongst themselves. However, as indicated by the upper-left and lower-right regions, the transferability between even donors and odd acceptors, and vice versa is poor.

Eager to take adavantage of this correlation, I designed a metric that uses parity difference of donor-acceptor pairs to predict their transferability . The more similar the parities, the higher the predicted transferability. While this metric successfully predicted transferability for graph pairs in my dataset with a mean squared error of 0.0025, its failures were illuminating. In particular, it performed poorly on graph pairs which contained mixed parity graphs ($40-50\%$) as donors. For example, even though a mixed donor and an even acceptor have a large parity difference, they report high transferability. This is consistent with results in Figure 1 since mixed parity graphs only contain universally optimal parameters. Being transferable to any random graph, mixed parity graphs further illustrate the power of transferability.

Conclusions and Future Work

Transferability is a way to accelerate QAOA in solving the MaxCut problem. In this work, I showed that transferability can be explained and predicted from the parity of graphs. Yet, my analysis was limited in the size of graphs. While my preliminary findings suggests that the properties discussed above hold for donors as small as 4 nodes and acceptors as large as 64 nodes, a rigorous numerical study is lacking. Further, one may employ machine learning tools as well to predict transferability. In the future, my research group aims to address these concerns. I hope these findings present a pathway for speeding up quantum algorithms in solving graph optimization problems of social importance.

This work will be submitted to the journal *IEEE: Transactions on Quantum Engineering* for publication.

References

1. Piccini, J., Robledo, F. & Romero, P. Complexity among combinatorial problems from epidemics. *International Transactions in Operational Research* **25,** 295–318.
2. Fischetti, M., Fischetti, M. & Stoustrup, J. Safe distancing in the time of COVID-19. *European Journal of Operational Research* (2021).
3. Farhi, E., Goldstone, J. & Gutmann, S. *A Quantum Approximate Optimization Algorithm* 2014. arXiv: 1411.4028 [quant-ph].
4. Galda, A., Liu, X., Lykov, D., Alexeev, Y. & Safro, I. Transferability of optimal QAOA parameters between random graphs. *2021 IEEE International Conference on Quantum Computing and Engineering* (2021).
5. Lykov, D., Schutski, R., Galda, A., Vinokur, V. & Alexeev, Y. *Tensor Network Quantum Simulator With Step-Dependent Parallelization* 2020. arXiv: 2012.02430 [quant-ph].