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Variational Quantum Eigensolver algorithm to find excited states of a Hamiltonian

My research this summer was in the field of quantum cognition, under the mentorship of Professor Bhattacharjee Abhishek and Dr. Pothukuchi Raghav. Quantum cognition refers to the use of quantum computing methods and ideas to tackle problems in cognitive science. One of the possible advantages of using quantum computers over classical computers is that performance scales well in some problems like optimization, where we need to consider a landscape of many possible outcomes. This summer research is a continuation of my work with Prof. Bhattacharjee's group since Fall 2020. During the past academic year, I explored the use of quantum random walks and started work on a Variational Quantum Eigensolver (VQE) in Qiskit, a quantum programming toolkit based on Python. The original VQE algorithm finds the lowest energy state of a Hamiltonian system. The goal of my summer research was to extend this implementation, by achieving a closer match with the known theoretical minimum energy value as well as seek the next few lowest energy states. The motivation of our project was to develop a package to generate well-defined wave functions in Qiskit, which are useful in various cognitive science models.

The hypothesis tested is that the Variational Quantum Eigensolver and its Subspace Search variant may be able to generate accurate energy state functions, based on appropriate Hamiltonian, quantum "ansatz" circuit and classical optimization algorithm choices. The parameters of the model were tested so as to find the best, most efficient design.

The VQE algorithm is a quantum computing approach to minimize the expectation value of a parameterized quantum circuit, also known as an "ansatz", using a hybrid quantum-classical feedback loop. The quantum ansatz circuit consists of various quantum gates that are adjustable in each iteration; the iterations depend on a classical computer algorithm. By changing the gates, VQE aims to transform an input quantum state to the lowest energy state with the lowest expectation value upon measurement. Hence, determining an ideal quantum ansatz and classical optimization loop are two key questions for this research.

A new modification to the VQE is the Subspace Search VQE (SSVQE), which expands on the VQE ansatz by prepending an additional ansatz component to search within a subspace of input vectors. The SSVQE is a popular method to find more states beyond the lowest ground state. Compared to the VQE which minimizes only one input's expected outcome, the SSVQE considers a weighted sum of multiple inputs' outcomes. For example, we map |0000>, |0001>, |0010> and |0011> input wave states to the first, second, third and fourth energy states respectively. In this process, the weight's role is to assign the correct output energy to the respective input. This ability will be important when applying the VQE method to scientific problems of interest, for example in simulating chemical reactions. During the summer, I successfully extended my VQE program to the SSVQE method. Hence, in one single optimization step we could generate an ansatz to reach the ground, second, third and fourth energy states.

In terms of the classical optimization, I tried various algorithms and eventually found three types suitable for optimizing a quantum circuit problem. The three are: Constrained Optimization by Linear Optimization (COBYLA), Simultaneous Perturbation Stochastic Approximation (SPSA) and Nelder Mead. I found that the gradient-free COBYLA gave the fastest results, but could not operate at the level of detail required for teasing out the lowest energy states. SPSA worked the best, however it took a lot more iterations to complete compared to COBYLA or Nelder Mead.

For the ansatz design, I started off with a comprehensive two qubit, eight U3 gate ansatz which was able to reach all possible two qubit quantum states. However, this ansatz layout does not scale well as we increase qubit

numbers. After doing more literature review, I found a “hardware-efficient” ansatz design that uses fewer gates and scales well to three or four qubit wires. The hardware-efficient ansatz in addition lets us fine-tune computational performance in terms of the number of entanglement layers. I found that the more entanglement layers used, the more accurate the output wave function, yet the longer time it takes for the classical (SPSA) optimizer to cover all possibilities. In the current stage, we believe a ten entanglement layer with a setting of 5000 iterations with the SPSA optimizer yields good results for finding the first, second, third and fourth energy states together under the SSVQE algorithm.

One difficulty was getting an accurate cost function to tally with the ground state. Since the Hamiltonian selected was that of a standard potential well function, we know the ideal ground state energy (also equal to the Hamiltonian matrix’s lowest eigenvalue) is 0.049. After checking the code for the cost function, I managed to resolve this issue and aligned the numerical minimum energy found to equal the theoretical ground state energy. This matched our physical understanding of the potential well system, and allowed us to move on to finding the next higher states. While the theoretical energy state multiples should be 1x, 4x and 9x for the first, second and third energy states (with respect to the first state), I could obtain values around 2x, 4x and 12x with the SSVQE ansatz. More accurate matches can be found by allowing the computer to run even more iterations.

Through the course of this research, I further developed my understanding of quantum physics and computing principles, programming in Qiskit and the problem scoping for scientific research. There were many parameters involved in this project, ranging from ansatz design to optimization parameters to algorithm use, and figuring out how to systematically explore them was an important step.

While this summer my research was fully remote and done from home, I received excellent support from Prof. Bhattacharjee, Dr. Pothukuchi and the research group through weekly calls and email discussions. We plan to include my VQE work this summer under the Fellowship in a future paper on quantum cognition.

This Fellowship opportunity has let me further learn about quantum computing and physics. We were able to dive deeper into my earlier results, and understand the intricacies of the VQE and SSVQE algorithms. After this summer, I intend to continue research with Prof. Bhattacharjee and Dr. Pothukuchi to apply the developed base-states program to cognitive science models. I am also going to take further advanced courses in Physics the next two years, including Classical Mechanics and Quantum Mechanics. The Fellowship research program has highlighted areas of improvement for me as a future quantum computing researcher.

I am thankful for the sponsors of the Yale College Dean’s Research Fellowship in the Sciences, which has allowed me to spend a fruitful and interesting summer doing research.