Variational Quantum Eigensolver – SQUANDER
- Report 4. -

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1 Variational Quantum Eigensolver

The Variational Quantum Eigensolver (VQE) is a hybrid algorithm that combines both quantum and classical computation [1] to estimate the ground state energy of quantum systems [2]. It works by employing a parameterized quantum circuit to create trial wavefunctions, while a classical optimization routine iteratively reduces the expected value of the Hamiltonian.

2 Hamiltonian generation process

To run simulations, we need the Hamiltonian. It can be given exactly, but it is more precise if we generate the matrix explicitly. Initially, we need to create a topology, which can be represented as a random regular graph. The `networkx` package provides a function suitable for this purpose[1]. This function generates a random d-regular graph on n nodes, where n corresponds to the number of qubits in our case. By providing a seed value, we can ensure the generation is reproducible. Finally, the random graph is modified to implement the XXX Heisenberg model.

3 Results

I generated the datasets with the corresponding degree values ($d \in 2, 3, 4$). For this part of the semester project, I used the *ADAM*, *Powell*, and *Batched Line Search* optimization methods. The results are presented in the following.

Figure 1, Figure 3, and Figure 5 illustrate the randomly generated graphs used in the simulations for $d = 2$, $d = 3$, and $d = 4$, respectively. These graphs represent the structure of the problem instances for each degree value, where the nodes correspond to variables and the edges indicate constraints or dependencies.

Figures 2, 4, and 6 show the performance of the optimization methods on these graphs. The vertical axis in each plot represents the minimized energy, and the horizontal axis denotes the number of cost function evaluations. As seen in all three plots, the *Batched Line Search* method consistently achieves faster convergence and lower minimal energy compared to the other two methods as shown in early reports. The *Powell* method performs moderately well, while *ADAM* shows the slowest convergence, especially as the degree d increases.

[1] See: networkx.org/random_regular_graph

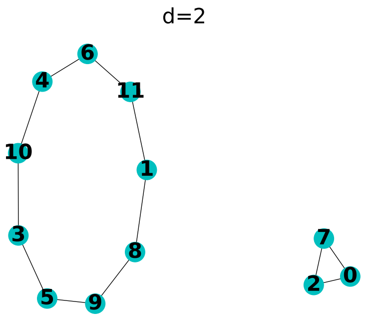

Figure 1: The random graph of the simulation.

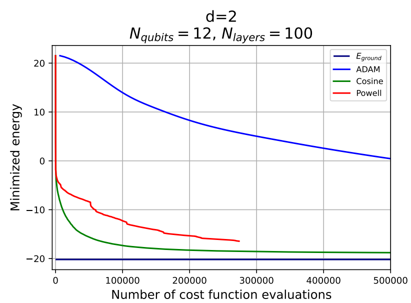

Figure 2: Simulations with $d = 2$.

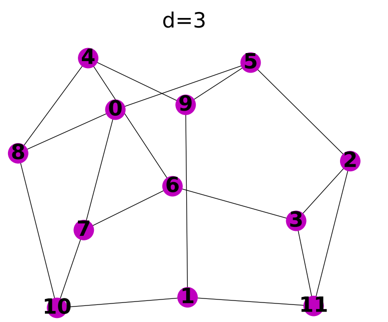

Figure 3: The random graph of the simulation.

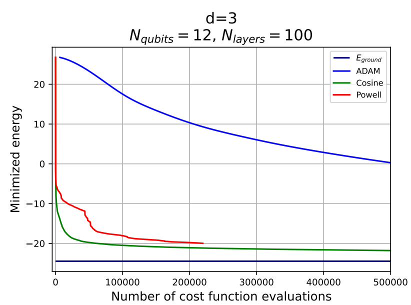

Figure 4: Simulations with $d = 3$.

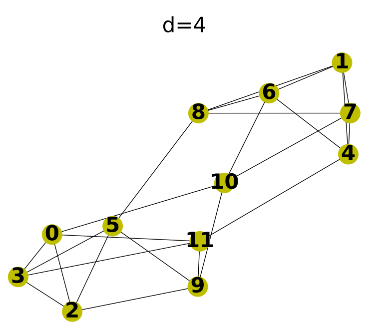

Figure 5: The random graph of the simulation.

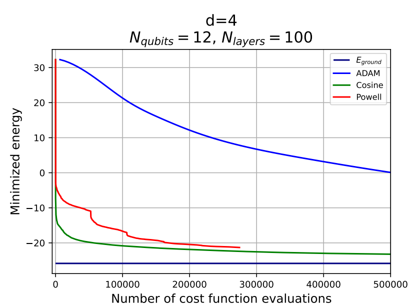

Figure 6: Simulations with $d = 4$.

For additional results and codes, visit my GitHub[2] page, a forked version of SQUANDER.

4 Future plans

Over the next two weeks, I plan to change the *random seed* parameter used for generating the random regular graph in the Hamiltonian. I will run simulations using the *ADAM*, *Powell*, and *Batched Line Search* optimization methods and evaluate their performance.

References

[1] Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik. *The theory of variational hybrid quantum-classical algorithms*. New Journal of Physics, 18(2):023023, 2016

[2] Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J Love, Alán Aspuru-Guzik, and Jeremy L O'brien. *A variational eigenvalue solver on a photonic quantum processor*. Nature communications, 5(1):4213, 2014

[2] https://github.com/menkobalazs/SMC-Lab-SQUANDER