Variational Quantum Eigensolver – SQUANDER - Report 3. -

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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 Optimization methods

The optimizations method of the VQE algorithm can be one of the following.

- **Gradient Descent:** This method iteratively updates the model parameters by moving in the direction of the negative gradient of the loss function, gradually approaching a local minimum.
- **Parameter Shift Rule** (also called Quantum Gradient Descent) [3]: This technique estimates gradients by evaluating quantum circuits at shifted parameter values, enabling gradient-based optimization in quantum machine learning.
- **ADAM** (Adaptive Moment Estimation) [4]: ADAM combines momentum and adaptive learning rates by keeping track of both first and second moments of the gradients, leading to fast and stable convergence.
- **BFGS** (Broyden–Fletcher–Goldfarb–Shanno) [5]: BFGS is a quasi-Newton method that builds an approximation to the inverse Hessian matrix to perform more informed and efficient parameter updates.
- **Powell's method** [6]: Powell's method performs optimization by iteratively minimizing the function along a set of conjugate directions, without requiring gradient information.
- **COBYLA** (Constrained Optimization BY Linear Approximation) [7]: COBYLA solves constrained optimization problems by constructing successive linear approximations of the objective and constraint functions.
- **Nelder–Mead** [8]: The Nelder–Mead algorithm minimizes functions using a simplex of points and transformations such as reflection, expansion, and contraction, making it useful for derivative-free optimization.
- **Batched Line Search Strategy** [9] (also called Cosine Strategy): This approach avoids the need for learning rate tuning by dynamically adapting the step size using cosine similarity, helping to prevent vanishing gradients and enabling traversal through narrow valleys.

3 Barren plateau problem

The barren plateau (BP) problem in VQE refers to the phenomenon where the gradient of the cost function vanishes exponentially with the size of the quantum system, making optimization extremely difficult. As a result, the parameter landscape becomes flat, and classical optimizers struggle to find a direction for improvement. This issue is particularly problematic in deep or unstructured quantum circuits, as it hinders the convergence of the algorithm and limits scalability. Understanding and mitigating barren plateaus is crucial for the practical implementation of VQE on larger quantum systems.

4 Result

Figure 1 shows the minimized energy as a function of the number of cost function evaluations. In all simulations, I used 10 qubits and 100 layers in the quantum circuit. To improve results, each simulation was initialized with a random parameter vector. It can be observed that both COBYLA and Powell's methods begin with relatively low energy values; however, COBYLA eventually gets stuck. After several thousand evaluations, the Cosine Strategy method outperformed the others by reaching the ground state energy with fewer evaluations of the cost function.

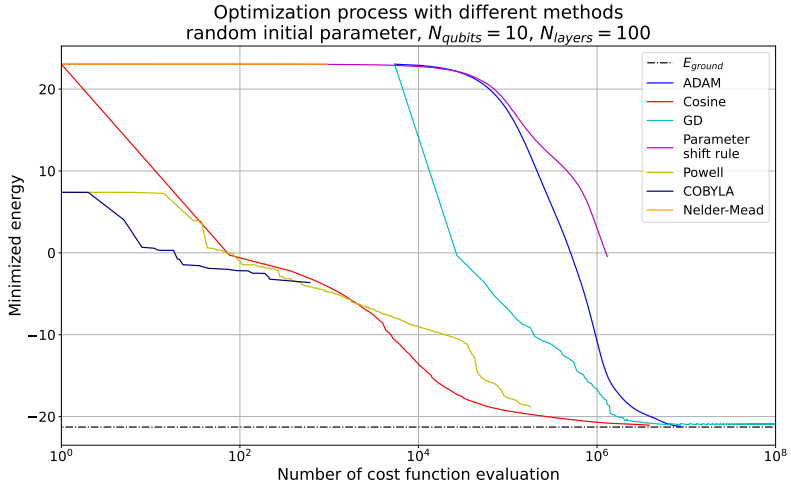

Figure 1: Simulations with different methods on logarithmic x scale.

The BP problem, as discussed in Section 3, can be observed when more qubits are used in the simulations, as shown in Figure 2. At 14 qubits, the Gradient Descent and BFGS method gets stuck on a barren plateau, preventing the minimization process from reaching the ground state energy.

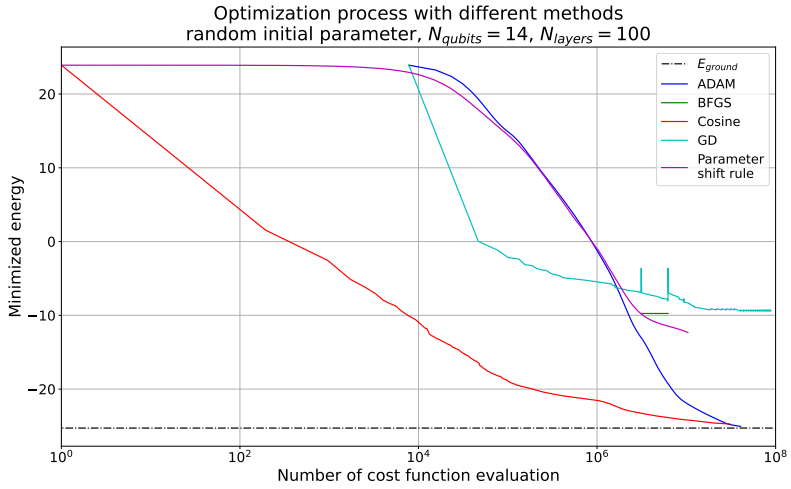

Figure 2: Simulations with different methods on logarithmic x scale.

For additional results and codes, visit my GitHub page: github.com/menkobalazs/SMC-Lab-SQUANDER, a forked version of SQUANDER.

5 Future plans

In the next two weeks, I plan to modify the degree of the random regular graph used to generate the Hamiltonian. I will run simulations using the *ADAM*, *Powell*, and *Batched Line Search* optimization methods and compare their performance.

References

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