Quantum Gate Synthesis – SQUANDER
- Report 2. -

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Variational Quantum Eigensolver

The Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical algorithm [1] used to approximate the ground state energy of quantum systems [2]. It leverages a parameterized quantum circuit to prepare trial wavefunctions and uses a classical optimizer to iteratively minimize the expectation value of the Hamiltonian.

Optimizing process

In my work, the Squander's *examples* folder was very helpful. My project is based on the `VQE/Heisenberg_VQE.py` file. In this source file, I made the following modifications:

- Added argument parsing to retrieve arguments from bash command lines.
- Modified the data-saving methods.
- Added three new optimizers, which are *gradient-free* methods.

Furthermore, I created a Python file to analyze the results of the simulations. In the next section, the results are presented.

Results of optimizations

Zero initial parameter vector

Basically the Python file used a vector contained only zeros as initial condition. On the Fig. 1. the minimization process over the number of cost function evaluation can be seen with five different gradient-based methods. Due to the initial vector the gradient descend based algorithms cannot work, the minima cannot be found. The situation is the same for the BFGS[1] method. In this case the Cosine method can find the minimal energy level then the ADAM method.

Random initial parameter vector

To solve the uprising problem, the randomization of initial parameter vector is solution. In the simulations I used a uniform distribution between $[0, 0.01]$. With this change I got Fig. 2. In this case the Cosine method performed as well as before, but the Gradient descend was the second except the bug that in two cases the minimized energy grew to 0. We discussed about it a little, but my project leader did not know the reason of this problem. The case of the Gradient descend with parameter shift rule method did not run well, it stopped before the minimization process finished. For the next presentation event I plan to run it again.

[1] Broyden–Fletcher–Goldfarb–Shanno algorithm, see an introduction here.

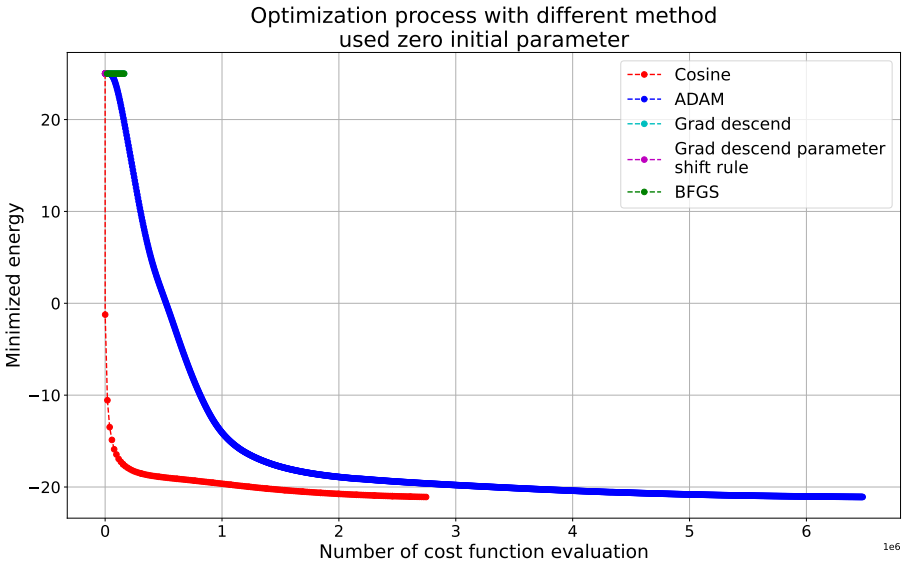

Figure 1: Minimization of cost function with zero initial parameters.

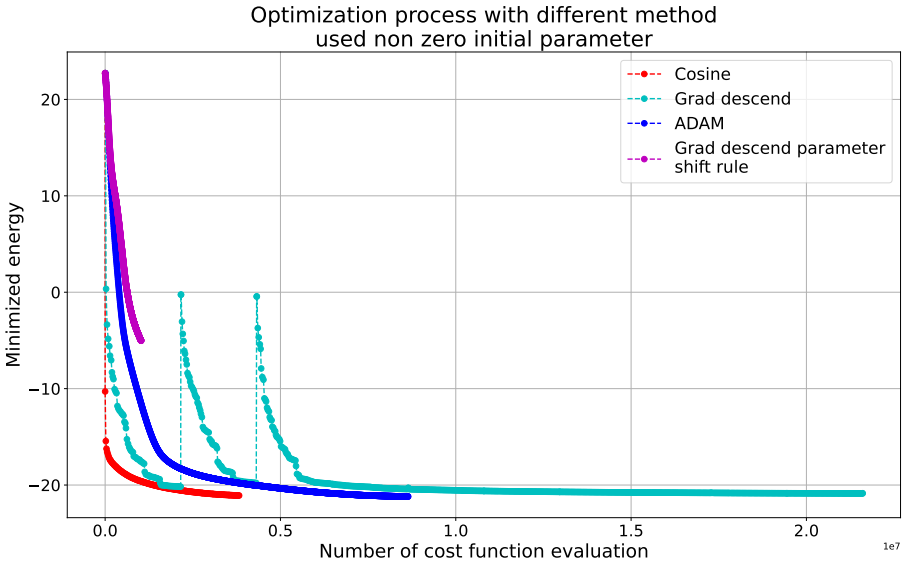

Figure 2: Minimization of cost function with random initial parameters.

Further plans

For the next presentation event I would like to create simulations with gradient-free methods and compare with the others.

As a further steps I would like to increase the number of circuit layers and the number of qubits to get more precise results. Then I am going to create more precise comparisons of the simulations.

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